JC18 Rec'd PCT/PTO 14 MAY 2001

FORM PTO-1390 (REV. 11-2000)

U.S. DEPARTMENT OF COMMERCE PATENT AND TRADEMARK OFFICE

TRANSMITTAL LETTER TO THE UNITED STATES DESIGNATED/ELECTED OFFICE (DO/EO/US) CONCERNING A FILING UNDER 35 U.S.C. 371

ATTORNEY 'S DOCKET NUMBER
54203-H-PCT-US/JPW/SHS

U.S. APPLICATION NO. (If known, see 37 CFR 1.5
09/856200

INTERNATIONAL APPLICATION NO.	INTERNATIONAL FILING DATE	PRIORITY DATE CLAIMED
PCT/US98/23905	10 November 1998	10 November 1997

TITLE OF INVENTION
CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120

APPLICANT(S) FOR DO/EO/US
Peter D. Kwong et al.

Applicant herewith submits to the United States Designated/Elected Office (DO/EO/US) the following items and other information:

1. [X] This is a **FIRST** submission of items concerning a filing under 35 U.S.C. 371.
2. [ ] This is a **SECOND** or **SUBSEQUENT** submission of items concerning a filing under 35 U.S.C. 371.
3. [ ] This is an express request to begin national examination procedures (35 U.S.C. 371(f)). The submission must include items (5), (6), (9) and (21) indicated below.
4. [X] The US has been elected by the expiration of 19 months from the priority date (Article 31).
5. [X] A copy of the International Application as filed (35 U.S.C. 371(c)(2))
   - a. [ ] is attached hereto (required only if not communicated by the International Bureau).
   - b. [ ] has been communicated by the International Bureau.
   - c. [X] is not required, as the application was filed in the United States Receiving Office (RO/US).
6. [ ] An English language translation of the International Application as filed (35 U.S.C. 371(c)(2)).
   - a. [ ] is attached hereto.
   - b. [ ] has been previously submitted under 35 U.S.C. 154(d)(4).
7. [X] Amendments to the claims of the International Aplication under PCT Article 19 (35 U.S.C. 371(c)(3))
   - a. [ ] are attached hereto (required only if not communicated by the International Bureau).
   - b. [ ] have been communicated by the International Bureau.
   - c. [ ] have not been made; however, the time limit for making such amendments has NOT expired.
   - d. [X] have not been made and will not be made.
8. [ ] An English language translation of the amendments to the claims under PCT Article 19 (35 U.S.C. 371 (c)(3)).
9. [ ] An oath or declaration of the inventor(s) (35 U.S.C. 371(c)(4)).
10. [ ] An English lanugage translation of the annexes of the International Preliminary Examination Report under PCT Article 36 (35 U.S.C. 371(c)(5)).

Items 11 to 20 below concern document(s) or information included:

11. [ ] An Information Disclosure Statement under 37 CFR 1.97 and 1.98.
12. [ ] An assignment document for recording. A separate cover sheet in compliance with 37 CFR 3.28 and 3.31 is included.
13. [X] A FIRST preliminary amendment.
14. [ ] A SECOND or SUBSEQUENT preliminary amendment.
15. [ ] A substitute specification.
16. [ ] A change of power of attorney and/or address letter.
17. [ ] A computer-readable form of the sequence listing in accordance with PCT Rule 13ter.2 and 35 U.S.C. 1.821 - 1.825.
18. [ ] A second copy of the published international application under 35 U.S.C. 154(d)(4).
19. [ ] A second copy of the English language translation of the international application under 35 U.S.C. 154(d)(4).
20. [ ] Other items or information:

JC18 Rec'd PCT/PTO 14 MAY 2001

U.S. APPLICATION NO. (If known, see 37 CFR 1.5)	INTERNATIONAL APPLICATION NO.	ATTORNEY'S DOCKET NUMBER
09/856200	PCT/US98/23905	54203-H-PCT-US/JPW/SHS

21. [X] The following fees are submitted:

BASIC NATIONAL FEE (37 CFR 1.492 (a) (1) - (5)):

	CALCULATIONS	PTO USE ONLY
Neither international preliminary examination fee (37 CFR 1.482) nor international search fee (37 CFR 1.445(a)(2)) paid to USPTO and International Search Report not prepared by the EPO or JPO **$1000.00**		
International preliminary examination fee (37 CFR 1.482) not paid to USPTO but International Search Report prepared by the EPO or JPO **$860.00**		
International preliminary examination fee (37 CFR 1.482) not paid to USPTO but international search fee (37 CFR 1.445(a)(2)) paid to USPTO **$710.00**		
International preliminary examination fee (37 CFR 1.482) paid to USPTO but all claims did not satisfy provisions of PCT Article 33(1)-(4) **$690.00**		
International preliminary examination fee (37 CFR 1.482) paid to USPTO and all claims satisfied provisions of PCT Article 33(1)-(4) **$100.00**		
ENTER APPROPRIATE BASIC FEE AMOUNT =	$ 710	
Surcharge of **$130.00** for furnishing the oath or declaration later than [ ] 20 [ ] 30 months from the earliest claimed priority date (37 CFR 1.492(e)).	$	

CLAIMS	NUMBER FILED	NUMBER EXTRA	RATE		
				$	
Total claims	32 - 20 =	12	x **$18.00**	$ 216	
Independent claims	13 - 3 =	10	x **$80.00**	$ 800	
MULTIPLE DEPENDENT CLAIM(S) (if applicable)			+ **$270.00**	$	
TOTAL OF ABOVE CALCULATIONS =				$ 1016	
[ ] Applicant claims small entity status. See 37 CFR 1.27. The fees indicated above are reduced by 1/2. +				$	
SUBTOTAL =				$ 1726	
Processing fee of **$130.00** for furnishing the English translation later than [ ] 20 [ ] 30 months from the earliest claimed priority date (37 CFR 1.492(f)).				$	
TOTAL NATIONAL FEE =				$ 1726	
Fee for recording the enclosed assignment (37 CFR 1.21(h)). The assignment must be accompanied by an appropriate cover sheet (37 CFR 3.28, 3.31). **$40.00** per property +				$	
TOTAL FEES ENCLOSED =				$ 0	
				Amount to be refunded:	$
				charged:	$

a. [ ] A check in the amount of $ ______________ to cover the above fees is enclosed.

b. [X] Please charge my Deposit Account No. 03-3125 in the amount of $ 1726 to cover the above fees. A duplicate copy of this sheet is enclosed.

c. [X] The Commissioner is hereby authorized to charge any additional fees which may be required, or credit any overpayment to Deposit Account No. 03-3125 . A duplicate copy of this sheet is enclosed.

d. [ ] Fees are to be charged to a credit card. **WARNING:** Information on this form may become public. **Credit card information should not be included on this form.** Provide credit card information and authorization on PTO-2038.

NOTE: Where an appropriate time limit under 37 CFR 1.494 or 1.495 has not been met, a petition to revive (37 CFR 1.137 (a) or (b)) must be filed and granted to restore the application to pending status.

SEND ALL CORRESPONDENCE TO:

John P. White, Esq.
Cooper & Dunham LLP
1185 Avenue of the Americas
New York, New York 10036

SIGNATURE

John P. White
Spencer Schneider
NAME

Reg. No. 28,678
Reg. No. 45,923
REGISTRATION NUMBER

09856200 .051402
09/856200
JC18 Rec'd PCT/PTO 14 MAY 2001

Dkt. 54203-H-PCT/JPW/SHS

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicants	:	Peter D. Kwong et al.
Serial No.	:	Not Yet Known (U.S. National Stage of PCT/US98/23905, filed 10 November 1998)
Filed	:	Herewith
For	:	CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120, COMPOUNDS INHIBITING CD4-gp120 INTERACTION, COMPOUNDS INHIBITING CHEMOKINE RECEPTOR-gp120 INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS

1185 Avenue of the Americas
New York, New York 10036
May 7, 2001

Assistant Commissioner for Patents
Washington, D.C. 20231

PRELIMINARY AMENDMENT

Please amend the subject application as follows:

In the specification:

On page 1, line 1, after the title, please delete the paragraph beginning "This application is a..." and insert the following paragraph:

--This application is a national stage entry filed under 35 U.S.C. §371 of PCT International Application No. PCT/US98/23905, filed November 10, 1998, which is a continuation-in-part and claims the benefit of U.S. Serial No. 09/100,631, filed June 18, 1998, U.S. Serial No. 09/100,763, filed June 18, 1998, U.S. Serial No. 09/100,529, filed June 18, 1998, U.S. Serial No. 09/100,762, filed June 18, 1998,

U.S. Serial No. 09/100,521, filed June 18, 1998 and claims the benefit of U.S. Serial No. 08/976,741, filed November 24, 1997, U.S. Serial No. 08/966,987, filed November 10, 1997, U.S. Serial No. 08/967,403, filed November 10, 1997, U.S. Serial No. 08/966,932, filed November 10, 1997, and U.S. Serial No. 08/967,148, filed November 10, 1997, the contents of which are incorporated by reference into this application.--

In the claims:

Please cancel claims 2-20, 22-26, 29-32, 35, 39-41, 43, 50-52, 54, 60, 62-79, 82, 87-89, 92-93, 95-96 without disclaimer or prejudice to applicants' right to pursue the subject matter of these claims in a later-filed application. Please amend claims 33, 44, 46, 55, 57, 90 and 94 under the provisions of 37 C.F.R. § 1.121(c) as follows. A marked up version of the amended claims wherein the deleted material is in brackets and the inserted material is underlined is attached hereto as **Exhibit 1.**

--33. (Amended) The compound identified by the method of claim 27.

--44. (Amended) The compound identified by the method of claim 37.

--46. (Amended) A composition comprising the compound of claim 44 and a suitable carrier.--

--55. (Amended) The compound identified by the method of claim

48.--

--57. (Amended) A composition comprising the compound of claim 55 and a suitable carrier.--

--90. (Amended) A vaccine comprising the variant of claim 86.

--94. (Amended) An antibody against the variant of claim 86.

Remarks:

Claims 1-96 are pending in the subject application. Applicants have herein canceled claims 2-20, 22-26, 29-32, 35, 39-41, 43, 50-52, 54, 60, 62-79, 82, 87-89, 92-93, 95-96 without disclaimer or prejudice to applicants' right to pursue the subject matter of these claims in a later-filed application and amended claims 33, 44, 46, 55, 57, 90 and 94. This amendment does not involve any issue of new matter. Therefore, entry of this amendment is respectfully requested such that claims 1, 21, 27-28, 33-34, 36-38, 42, 44-49, 53, 55-59, 61, 80-81, 83-86, 90-91 and 94 will be pending.

If a telephone interview would be of assistance in advancing prosecution of the subject application, applicants' undersigned attorneys invites the Examiner to telephone either of them at the number provided below.

No fee, other than the $1,806.00 fee, which includes the $710.00 basic national fee and the $1,096.00 fee for additional claims is deemed necessary in connection with filing this Preliminary

Amendment and authorization is hereby given to charge this fee to Deposit Account No. 03-3125. If any additional fee is required, authorization is hereby given to charge the amount of any such fee to Deposit Account No. 03-3125.

Respectfully submitted,

John P. White
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EXHIBIT 1

--33. (Amended) The compound identified by the method of claim [32] 27.

--44. (Amended) The compound identified by the method of claim [43] 37.

--46. (Amended) A composition comprising the compound of claim 44 [or 45] and a suitable carrier.--

--55. (Amended) The compound identified by the method of claim [54] 48.--

--57. (Amended) A composition comprising the compound of claim 55 [or 56] and a suitable carrier.--

--90. (Amended) A vaccine comprising the variant of claim 86 [,87 or 88].

--94. (Amended) An antibody against the variant of claim 86 [,87 or 88].

09856200.010302 #9

Applicant or Patentee: Peter D. Kwong, et al. Attorney's
Serial or Patent No.: 09/856,200 Docket No: 54203-H-PCT-US
Filed or Issued: November 10, 1998 JPW/AJM/HA
Title of Invention or Patent: CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120 COMPOUND INHIBITING CD-4gp120 INTERACTION, COMPOUND INHIBITING CHEMOKINE RECEPTOR gp120 INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS

VERIFIED STATEMENT (DECLARATION) CLAIMING SMALL ENTITY STATUS UNDER 37 C.F.R. §1.9(f) AND §1.27(d) - NONPROFIT ORGANIZATION

I hereby declare that I am an official empowered to act on behalf of the nonprofit organization identified below:

Name of Organization: The Trustes of Columbia University In the City of New York
Address of Organization: Broadway and West 116th Street New York, New York 10027

TYPE OF ORGANIZATION:

X UNIVERSITY OR OTHER INSTITUTION OF HIGHER EDUCATION
___ TAX EXEMPT UNDER INTERNAL REVENUE SERVICE CODE 26 U.S.C. §§501(a) and 501(c)(3)
___ NONPROFIT SCIENTIFIC OR EDUCATIONAL UNDER STATUTE OF STATE OF THE UNITED STATES OF AMERICA
NAME OF STATE: ___
CITATION OF STATUTE: ___
___ WOULD QUALIFY AS TAX EXEMPT UNDER INTERNAL REVENUE SERVICE CODE 26 U.S.C. §§501(a) and 501(c)(3) IF LOCATED IN THE UNITED STATES OF AMERICA
___ WOULD QUALIFY AS NONPROFIT SCIENTIFIC OR EDUCATIONAL UNDER STATUTE OF STATE OF THE UNITED STATES OF AMERICA IF LOCATED IN THE UNITED STATES OF AMERICA
NAME OF STATE: ___
CITATION OF STATUTE: ___

I hereby declare that the nonprofit organization identified above qualifies as a nonprofit organization as defined in 37 C.F.R. §1.9(e)* for purposes of paying reduced fees under 35 U.S.C. §41(a) and 41(b), with regard to the invention entitled CRYSTAL COMPRSING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120 COMPOUND INHIBITING CD4-gp120 INTERACTION, COMPOUNDS INHIBITING CHEMOKINE RECEPTOR gp120 INTERACTION, MIMICS OF CD4-gp120 VARIANTS
by inventor(s) Peter D. Kwong, Wayne A. Hendrickson, Joseph G. Sodroski, Richard T. Wyatt
described in:

___ the specification filed herewith
X application serial no. 09/856,200 filed November 10, 1998
___ patent no. ___ issued ___

I hereby declare that rights under contract or law have been conveyed to and remain with the nonprofit organization with regard to the above identified invention.

If the rights held by the nonprofit organization are not exclusive each individual, concern, or organization known to have rights to the invention is listed below[a] and no rights to the invention are held by any person, other than the inventor, who could not qualify as a small business concern under 37 C.F.R. §1.9(d)* or a nonprofit organization under 37 C.F.R. 1.9(e)*

[a]NOTE: Separate verified statements are required from each person, concern, or organization having rights to the invention averring to their status as small entities. 37 C.F.R. §1.27.

Name: ___
Address: ___

___ Individual ___ Small Business Concern ___ Nonprofit Organization

*See Reverse

Small Entity/Nonprofit
Page -2-

I acknowledge the duty to file, in this application or patent, notification of any change in status resulting in loss of entitlement to small entity status prior to paying, or at the time of paying, the earliest of the issue fee or any maintenance fee due after the date on which status as a small entity is no longer appropriate. 37 C.F.R. §1.28(b)*.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under 18 U.S.C. §1001, and that such willful false statements may jeopardize the validity of the application, any patent issuing thereon, or any patent to which this verified statement is directed.

Name of Person Signing: Michael J. Cleare, Ph.D.
Title In Organization: Executive Director - Columbia Innovation Enterprise
Address: Columbia University, Engineering Terrace - Suite 363
Amsterdam Avenue & West 120th Street, New York, New York 10027
Signature: MJ Cleare
Date Of Signature: 12/20/02

*See Reverse

CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120, COMPOUNDS INHIBITING CD4-gp120 INTERACTION, COMPOUNDS INHIBITING CHEMOKINE RECEPTOR-gp120 INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS

This application is a contiunation-in-part of U.S. Serial No. 09/100,631, filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/976,741, filed November 24, 1997, U.S. Serial No. 09/100,763, filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/966,987, filed November 10, 1997, U.S. Serial No. 09/100,529, filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/967,403, filed November 10, 1997, U.S. Serial No. 09/100,762, filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/966,932, filed November 10, 1997, U.S. Serial No. 09/100,521, filed June 18, 1998 a continuation-in-part of U.S. Serial No. 08/967,148, filed November 10, 1997. The contents of the above-identified application are incorporated into this application by reference.

The invention disclosed herein was made with United States Government support under National Institute of Health Grant Nos. Al 31783, Al 39420, Al 28691, CA 06516, Al 41851, Al 40895, GM 5-20394 and CUID 511168. Accordingly, the United States Government has certain rights in this invention.

Various references are referred to within this application. Disclosures of these publications in their entireties are hereby incorporated by reference into this application to more fully describe the state of the art to which this invention pertains.

Background of the Invention

During the first thirty years of protein

crystallization, the standard conceptual practice was to treat the protein as a fixed constant and screen it through a multitude of crystallization conditions. Advances in this approach has led to the development of crystallization robots capable of testing thousands of conditions (1,2). While this approach has had success, it fails for many interesting proteins.

One of these is the Human Immunodeficiency Virus (HIV)-1 envelope glycoprotein, gp120. HIV induces acquired immunodeficiency syndrome (AIDS) in humans (3,4). The gp120 glycoprotein helps to mediate virus entry into cells through sequential recognition of two cellular receptors of the human host, CD4 (5,6), and a chemokine receptor (primarily CXCR-4 or CCR-5, depending on viral strain) (7-12). These high affinity interactions are attractive targets for mimetic drug design. Although the structure of the gp120-binding domain of CD4 and the identity of residues critical to its interaction with gp120 have been known for several years (13,14), this has not been sufficient for design of potent antagonists (15-17). As the major virus-specific antigen accessible to neutralizing antibodies, knowledge of the gp120 structure could also impact considerably on vaccine design.

The gp120 protein has been an obvious target for structural investigation, and quantities of pure soluble protein have been available for several years, a byproduct in part from vaccine trials. Nevertheless, despite considerable effort, it has resisted crystallographic analysis for more than a decade.

The mature gp120 glycoproteins of different HIV-1 strains have approximately 470-490 amino acids (18).

Extensive N-linked glycosylation at approximately 20-25 sites accounts for roughly half its mass (18,19). Sequences from many different viral isolates show that it contains five conserved regions (C1-C5) and five variable regions (V1-V5) (18, 20) and nine conserved disulfide bridges (19). Except for limited N- and C-terminal cleavage, proteolytic digestion does not reveal a sub-domain structure. Indeed, even after extensive proteolytic cleavage, the unreduced protein runs near its native molecular weight on SDS-PAGE (Peter D. Kwong: unpublished data). Some of the variable regions, the V3 loop in particular, appear to be conformationally variable. Conformational change is also evidenced by shedding, the CD4-induced dissociation of gp120 from the surface of the virus, and by ligand-induced variations in monoclonal antibody binding (21,22). These changes may be related to the functional role of gp120 in virus entry.

The extensive glycosylation and conformational heterogeneity of gp120 suggested that merely screening the protein through ever more exotic crystallization conditions would not produce well-diffracting crystals. We therefore adopted a fundamentally different approach, which we term variational crystallization. This approach employed on radical modification of the protein surface, primarily to reduce heterogeneity, but also as a means of varying potential crystallization lattice contacts. An interactive cycle, involving different biochemical and molecular biological techniques, was used to detect and remove chemical and conformational heterogeneity. In addition, protein ligands, such as CD4 and the Fabs of monoclonal antibodies, were used to restrict conformational mobility. Progressive trials of 18 different gp120 crystallization variants yielded six

different crystals. This paradigm of crystallization, with a focus on protein modification rather than on crystallization screening, may aid in the structural analysis of other conformationally complex proteins.

Summary of the Invention

The subject invention provides a crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120, wherein the amino acid sequence is at least 100 amino acids in length.

The subject invention also provides the above-described crystals, which effectively diffract X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 2.5 angstroms or better than 2.5 angstroms.

The subject invention also provides the above-described crystals, wherein the crystal is arranged in a space group $P222_1$, so as to form a unit cell of dimensions a=71.6 Å, b= 88.1 Å, c=196.7 Å, and which effectively diffracts x-rays for determination of the atomic coordinates of the gp120 to a resolution of 2.5 Å or better.

The subject invention additionally provides a method for producing a crystal suitable for X-ray diffraction comprising: (a) deglycosylating a polypeptide having amino acid sequence of a portion of a gp120 wherein said portion is produced by deleting or replacing part of the gp120 to reduce the surface loop flexibility; (b) contacting the polypeptide with a ligand so as to form a complex which exhibits restricted conformational mobility; and (c) obtaining crystal from the complex so formed to produce a crystal suitable for X-ray diffraction.

The subject invention also provides the above-described methods, wherein the V1, V2, or V3 loop of the gp120

contained in the polypeptide are partially truncated, deleted or replaced.

The subject invention also provides a method for identifying a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and (b) determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the gp120.

This invention also provides a method of inhibiting the interaction of HIV-gp120 with CD4 which comprises administering to a mammal in need thereof a compound capable of disrupting two or more of the contacts between gp120 and CD4 as set forth in Figure 54.

This invention also provides a method for identifying a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and (b) determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the CD4 binding site of the gp120.

This invention also provides a method for designing a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120

comprising: (a) determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and (b) designing a compound to fit the CD4 binding site.

This invention also provides a method of inhibiting Human Immunodeficiency Virus infection in a subject comprising adminstering effective of amount of the above-described composition to the subject.

This invention provides a method for identifying a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and (b) determining whether a compound would fit into the binding site, a positive fit indicating that the compound is capable of binding to the chemokine receptor binding site of the gp120.

This invention also provides a method for designing a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and (b) designing a

compound to fit the chemokine receptor binding site.

This invention also provides the above-described methods, wherein the crystal further comprises a chemokine receptor, a second polypeptide having amino acid sequence of a portion of chemokine receptor, an antibody or a Fab capable of binding to the chemokine receptor binding site or a compound known to be capable of binding to the chemokine receptor binding site, bound to the polypeptide.

This invention further provides a method of inhibiting the interaction of HIV-gp120 with chemokine receptor which comprises administering to a mammal in need thereof a compound capable of disrupting two or more of the contacts between gp120 and chemokine receptor as set forth in Figure 55, thereby inhibiting the interaction of HIV-gp120 with chemokine receptor.

This invention provides a substance mimicking the gp120-binding domain of CD4 wherein the size of the residue or analog thereof at position 43 is bigger than the size of a phenylalanine so as to increase the affinity for human immunodeficiency virus envelope glycoprotein gp120.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 10 Å across its longest dimension.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof, wherein the residue's longest dimension is longer than phenylalanine's longest dimension.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 15 Å across its longest dimension.

This invention also provides the above-described substances, wherein the modification involves replacemnet of the residue at position 43 with a cysteine.

This invention also provides the above-described substances, wherein the modification involves replacement of the residue at position 43 with a tyrosine.

This invention further provides a pharmaceutical composition capable of inhibiting cell entry by HIV, comprising (a) an effective amount of the substance of claim 1; and (b) a pharmaceutically acceptable carrier.

This invention further provides a method of inhibiting cell entry by HIV, comprising contacting the cells with an effective amount of the above-described substances, thereby inhibiting cell entry by HIV.

This invention further provides a method of treating or preventing HIV infection in a subject, comprising administering to the subject an effective amount of the above-described substances, thereby treating or preventing HIV infection.

The subject invention provides a variant of gp120 which presents a hidden, conserved, neutralization epitope.

The subject invention also provides a composition

comprising a variant of gp120 which presents a hidden, conserved, neutralization epitope and a suitable carrier.

The subject invention further provides a vaccine comprising a variant of gp120 which presents a hidde conserved, neutralization epitope and a suitable carrier.

The subject invention also provides an antibody induced by a vaccine comprising a variant of gp120.

Brief Description of the Figures

Figures for the First Series of Experiments

Figure 1

Computer-generated ribbon drawing of the tertiary structure of CD4, gp120, and Fab 17b interacting. CD4 is in the top left, gp120 is toward the right, and Fab 17b is in the bottom left of the figure.

Figure 2

Illustration of the locations of CD4, gp120, and Fab 17b in the computer-generated ribbon drawing of figure 1.

Figure 3

Photomicrographs of crystals containing HIV-1 gp120. Crystal types A-F are shown and correspond to the crystal types described in the text and Tables 3 and 4. The photomicrograph in A is at twice the magnification. The bar in A corresponds to 25 μm (50 μm for B-F).

Figure 4

Polyacrylamide gel electrophoresis (PAGE) of the ternary complex crystals (Type E). A cluster of crystals (0.4x0.1x0.05mM) was washed four times with 1 μl of reservoir solution and dissolved in 3 μl of loading buffer and analyzed by SDS-PAGE on a 8-25% gradient gel (Pharmacia Phast system). Lane 1, 2.5 ug of ternary complex purified by gel filtration. The top band is the deglycosylated Δ82ΔV1/2*ΔV3ΔC5 gp120, the next two bands are the alkylated and reduced heavy and light chains respectively of the Fab 17b, and the bottom band is the two-domain sCD4 (D1D2). Lane 2, standards: 94, 67, 43 (diffuse), 30, 20, and 14. Lane 3, supernant from the crystallization droplet. Lane 4, last wash of crystals. Lane 5, dissolved crystals. The gel is silver stained.

Figure 5 A and B

Crystals formed under condition one described in Table 7.

Figure 6

Crystals formed under condition two described in Table 7.

Figure 7

Crystals formed under condition three described in Table 7.

Figure 8

Crystals formed under condition four described in Table 7.

Figure 9

Crystals formed under condition five described in Table 7.

Figure 10

Crystals formed under condition six described in Table 7.

Figure 11

Crystals formed under condition seven described in Table 7.

Figure 12

Crystals formed under condition eight described in Table 7.

Figure 13

Crystals formed under condition nine described in Table 7.

Figure 14

Crystals formed under condition ten described in Table 7.

Figure 15

Crystals formed under condition eleven described in Table 7.

Figure 16

Crystals formed under condition twelve described in Table 7.

Figure 17

Crystals formed under condition thirteen described in Table 7.

Figure 18

Crystals formed under condition fourteen described in Table 7.

Figure 19

Crystals formed under condition fifteen described in Table 7.

Figure 20

Crystals formed under condition sixteen described in Table 7.

Figure 21

Crystals formed under condition seventeen described in Table 7.

Figure 22

Crystals formed under condition eighteen described in Table 7.

Figure 23

Crystals formed under condition nineteen described in Table 7.

Figure 24

Crystals formed under condition twenty described in Table 7.

Figure 25

Crystals formed under condition twenty-one described in Table 7.

Figures for the Second Series of Experiments

Figures 26A and 26B

The HIV-1 entry process. The trimeric HIV-1 envelope glycoproteins, anchored in the viral membrane, are depicted, with gp120 in the lower right and gp41 in the upper right. For simplicity, the gp120 variable loops are not shown, but would extend over the outer surface of the envelope glycoprotein complex. The receptors on the target cell, CD4 and chemokine receptor, are also shown. The structures of gp120, gp41, and CD4 are

adapted from available X-ray crystallographic studies (5,20,21), whereas the chemokine receptor model is hypothetical.

<u>Figure 27</u>

The HIV-1 gp120 surface.

<u>Figure 27A</u>

The molecular surface of the HIV-1 gp120 core (20) is shown, with the arrow pointing towards the viral membrane. The inner domain, believed to interact with gp41, and the outer domain, which is probably exposed on the assembled trimer, are on the left and right, respectively. The gp120 surface occluded by CD4 is shown and the gp120 region thought to be involved in chemokine receptor binding (27) is also shown. The location of the base of the V3 loop is shown.

<u>Figure 27B</u>

Conserved gp120 neutralization epitopes are shown on the gp120 core, which is oriented identically to that in Figure 16A. The location of the epitopes was deduced from mutagenic analysis (45,46,48).

<u>Figure 27C</u>

The approximate location of gp120 structures (20) that contribute to protection from antibody responses is shown. The major variable loops (V2, V3, and V4), the V5 region and the sites of N-linked glycosylation are shown.

<u>Figure 16D</u>

The relationship of different surfaces of the gp120 core to the antibody response generated by the gp120 glycoprotein is depicted. The surface of gp120 that interacts with neutralizing antibodies (32) is shown, spans the inner and outer domains, and includes the V2 and V3 variable loops (not shown). The surface of gp120 that interacts with non-neutralizing antibodies is located on the inner domain, and includes gp41-

interactive N- and C-terminal gp120 regions (not shown). The heavily glycosylated surface of the gp120 outer domain, which appears to be minimally immunogenic, is also shown.

Figures for the Third Series of Experiments

Figure 28

Overall structure. The ribbon diagram shows gp120, the N-terminal two domains of CD4, and the Fab 17b (light chain) and (heavy chain). The sidechain of Phe 43 on CD4 is also shown. The prominent CDR3 loop of the 17b heavy chain is evident in this orientation. Although the complete N- and C- termini of gp120 are missing, the positions of the gp120 termini are consistent with the proposal that gp41, and hence the viral membrane, is located towards the top of the diagram. This would position the target membrane at the diagram base. The vertical dimension of gp120 in this orientation is roughly 50 Å. Precisely perpendicular views of gp120 are shown in Figures 29 and 30. Drawn with RIBBONS[49].

Figure 29

Structure of core gp120. The orientation of gp120 in each of the panels shown in this figure is related to Figure 17 by a 90^0 rotation about a vertical axis. Thus the viral membrane would be oriented above, the target membrane below, and the C-terminal tail of CD4 coming out of the page. In this view, we describe the left portion of core gp120 as the "inner" domain, the right portion as the "outer" domain, and the 4-stranded sheet at the bottom left of gp120 as the "bridging sheet." The bridging sheet (β3, β2, β21, β20) can be seen packing primarily over the inner domain, although some surface residues of the outer domain, e.g. Phe 382, reach in to form part of its hydrophobic core.

Figure 29A

Ribbon diagram. Helices and β-strands are depicted. strand β15 makes an antiparallel β-sheet alignment with strand C'' of CD4. The dashed line to the right of the diagram represents the disordered V4 loop. Selected parts of the structure are labeled.

Figure 29B

Secondary structure diagram. The schematic is arranged to coincide with the orientation of Figures 29A and 29C. Helices are shown as corkscrews and labeled α1-α5. β-strands are shown as arrows: black and labeled represent the 25 β-strands of core gp120; gray and unlabeled represent the continuation of hydrogen bonding across a sheet; white and labeled represents the C'' strand of CD4. Spatial proximity between neighboring strands implies mainchain hydrogen bonding. Loops are labeled ζA-ζF and V1-V5. The labels of loops with high sequence variability are circled. Assignment of secondary structure was accomplished with the Kabsch and Sander algorithm except for β4 and β8, which are both interrupted mid-strand by sidechain-backbone hydrogen bonds, β9, β15, and β25a, all of which have angles or hydrogen bonds which are slightly non-standard, and α4, which hydrogen bonds as a 3-10 helix with the final residue in β-conformation.

Figure 29C

Stereo plot of an α-carbon trace. Every 10th Cα is marked with a filled circle, and every twentieth residue is labeled. Disulfide connections are depicted as ball and stick. Shown are ordered residues, 90-396 and 410-492.

Figure 29D

Structure-based sequence alignment. Shown are the sequences of "HIV-1 B" (core gp120 from clade B, strain HXBc2 used in these studies), "C"(HIV-1 clade C, strain UG268A2), "O"(HIV-1 clade O, strain ANT70),

"HIV-2"(strain ROD), and "SIV"(African green monkey isolate, clone GRI-1). The secondary structure assignments are shown as arrows and cylinders, with (x) denoting residues which are disordered in the present structure. The "gars" sequence at the N-terminus and the "gag" sequence in the V1/V2 and V3 loops are consequences of the gp120 truncation. Solvent accessibility is indicated for each residue by an open circle if the fractional solvent accessibility is greater than 0.4, a half-closed circle if 0.1 to 0.4, and a closed circle if less than 0.1. Sequence variability observed among primate immunodeficiency viruses is indicated below the solvent accessibility by the number of horizontal hash marks: 1 mark, residues conserved among all primate immunodeficiency viruses; 2 marks, conserved among all HIV-1 isolates; 3 marks, exhibits moderate variation among HIV-1 isolates; and 4 marks, exhibits significant variability among HIV-1 isolates. In accessing conservation, all single atom changes were permitted as well as larger substitutions if the character of the sidechain was conserved (e.g. K to R or F to L). N-linked glycosylation is indicated by "m" for the high mannose additions and "c" for the complex additions observed in mammalian cells (6). Residues of gp120 in direct contact with CD4 are indicated by "*". Direct contact is a more restrictive criterion of interaction than the often used loss of solvent accessible surface; residues of gp120 which show loss of solvent accessible surface but are not in direct contact are 123, 124, 126, 257, 278, 282, 364, 471, 475, 476 and 477. Parts (a) and (b) were drawn with MOLSCRIPT (P. J. Kraulis).

Figure 30

CD4-gp120 interactions.

Figure 30A

Ribbon diagram of gp120 binding to CD4. Residue Phe 43 of CD4 is also depicted reaching into the heart of gp120. From this orientation the recessed nature of the gp120 binding pocket is evident.

Figure 30B

Electron density in the Phe 43 cavity. The 2Fo-Fc electron density map at 2.5Å, 1.1σ contour, is shown. The orientation is the same as in (a). The foreground has been clipped for clarity removing the overlying β24-α5 connection. In the upper middle of the picture is the central unidentified density. At the bottom of the picture, Phe 43 of CD4 can be seen reaching up to contact the cavity. Moving clockwise around the cavity, the gp120 residues are Trp 427 (with its indole ring partially clipped by foreground slabbing), Trp 112, Val 255, Thr 257, Glu 370 (packing under the Phe 43 ring), Ile 371, and Glu 368 (partially clipped in the bottom right corner). Hydrophobic residues lining the back of the cavity can be partially glimpsed around the central unidentified density.

Figure 30C

Electrostatic surface of CD4 and gp120. The electrostatic potential is displayed at the solvent accessible surface, which is shaded according to the local electrostatic potential. The slight "puffiness" of the surface arises from the enlarged nature of the solvent accessible surface relative to the standard molecular surface. On the right, the gp120 surface is shown in an orientation similar to that of Figures 29A and 29C, but rotated ~20^0 around a vertical axis to depict the recessed binding pocket more clearly. A thin yellow Cα worm of CD4 is shown to aid in orientation. On the left, the CD4 surface is shown, rotated relative to the gp120 panel by an exact 180^0 rotation about the vertical axis shown. A thin red Cα worm of gp120 is

shown.

Figure 30D

CD4-gp120 contact surface. On the right, the gp120 surface is shown with the surface within 3.5 Å of CD4 (surface-to-atom center distance). This effectively creates an "imprint" of CD4 on the displayed gp120 surface. On the left (180^0 rotation), the corresponding CD4 surface and gp120 "imprint" is also shown.

Figure 30E

CD4-gp120 mutational "hot-spots." On the right, the surface of gp120 is shown with the surface of gp120 residues shown by substitution to affect CD4 binding highlighted: substantial effect -- residues 257, 368, 370 and 427; moderate effect -- residue 457. Also depicted is the surface of the large water-filled cavity at the CD4-gp120 interface. On the left (180^0 rotation), residues important for gp120 binding are shown on the CD4 surface: substantial effect -- residues 43 and 59; moderate effect -- residues 29, 35, 44, 46, 47.

Figure 30F

Sidechain/mainchain contribution to the gp120 surface. The orientation is the same as the right panel of Figures 30C-30E, and below (Figure 30G), and allows for direct comparison of the CD4-gp120 contact surface. A striking surface concentration of mainchain atoms is seen in the regions corresponding to the CD4 "imprint."

Figure 30G

Sequence variability mapped to the gp120 surface. The sequence variability observed among primate immunodeficiency viruses (Figure 29D) is depicted mapped onto the gp120 surface. Also shown is the carbohydrate: N-acetylglucosamine and fucose residues present in the structure; Asn-proximal N-acetylglucosamines modeled at residues 88, 230, 241, 356, 397, 406, 462. Much of the carbohydrate (22 residues) is hidden on the back side of

the outer domain.

Figure 30H

Phe 43 cavity. The surface of the Phe 43 cavity is shown, buried in the heart of gp120. A worm representation of gp120 shows the three stretches that are incorrectly predicted by secondary structure prediction: the ζB loop, bending around the top of the cavity, strands β20-β21 just below the cavity, and strand β15, slightly more distal to the cavity right. The orientation shown here is the same as for the gp120 surfaces in Figure 30C-G.

Figure 30I

Schematic of the CD4-gp120 interface. This schematic of the entire interface shows six discrete segments of gp120 (solid black line) interacting with CD4 (double line). To aid in orientation, secondary structural elements are labeled, as are representative contact residues from each segment of gp120. Arrows indicate mainchain direction. The sidechain of Phe 43 is also shown. The orientation shown is similar to Figure 30A and 30B.

Figure 30J

Schematic of gp120 contacts around Phe 43 and Arg 59 of CD4. Residues on gp120 involved in direct contact with Phe 43 or Arg 59 are depicted. Electrostatic interactions are depicted as dashed lines. Hydrophobic interactions are found between Phe 43 (CD4) and Trp 427, Glu 370, Gly 473, and Ile 371 (all from gp120) and between Arg 59 (CD4) and Val 430 (gp120). The orientation is similar to Figure 30A, 30B, and 30I, but has been rotated for clarity. Sidechains of Phe 43 and Arg 59 as well as those portions of gp120 sidechains which interact with these crucial CD4 residues are drawn with bold lines.

(Figure 30A was drawn with RIBBONS[49], Figure 30B with the

program O[47], and Figures 30B-G with GRASP[50].)

Figure 31

Neutralizing antibody 17b-gp120 interface.

Figure 31A

Worm diagram of Fab 17b and gp120. The Fab 17b is shown binding to gp120. The orientation shown is the same as in Figures 29A and 29C.

Figure 31B

Contact surface and V3 loop. The surface of gp120 is shown with any surface within 3.5 Å of Fab 17b (surface-to-atom center) and the surface of the V3 base. The orientation is the same as in Figure 30A.

Figure 31C

Contact surface and V3 loop. The same as Figure 20B, but rotated around a horizontal axis to more clearly depict the 17b epitope.

Figure 31D

Electrostatic surface. The electrostatic potential is displayed at the solvent accessible surface, which is shaded according to the local electrostatic potential. The electrostatic shading is the same scale as that shown in Figure 30C. The surface that corresponds to the 17b epitope is the most electropositive region of the molecule. The V3 loop is truncated here, but sequence analysis shows that it is generally quite positively charged.

Figure 31E

Worm diagram of gp120. The gp120 is shown shaded according to the same scheme given in Figure 30A. The orientation is the same as in Figures 30C and 30D, that is, 90^0 from Figure 30A.

Figure 32

Schematic representation of the gp120 initiation of fusion. A single monomer of core gp120 is depicted in an orientation similar to Figures 29A and 29C. The "3"

symbolizes the 3-fold axis, from which gp41 interacts with the gp120 N- and C- termini to generate the functional oligomer. In the initial state of gp120 (on the surface of a virion), the V1/V2 loops are shown partially occluding the CD4 binding site. Following CD4 binding (now at a target cell, though above the glycocalyx), a conformational change is depicted as an inner/outer domain shift, with the dark circle denoting the formation of the Phe 43 cavity. This conformational change strains the interactions at the N- and C- termini of gp120 with the rest of the oligomer, priming the CD4-bound gp120 core. In the next step (which takes place directly adjacent to the target membrane), the chemokine receptor binds to the bridging sheet and the V3 loop (at the bottom left and right, respectively, of gp120), causing an orientational shift of core gp120 relative to the oligomer. This triggers further steps, which ultimately lead to the fusion of the viral and target membranes.

<u>Figure 33</u>

Structure of HIV-1 gp120 with neutralizing antibody and human receptor CD4.

Figures for the Fourth Series of Experiments

<u>Figure 34A</u>

Structure and orientation of the HIV-1 gp120 core. Cα tracing of the gp120 core, which was crystallized in a ternary complex with two-domain sCD4 and Fab fragment of the 17b antibody(12), is shown. The gp120 core is seen from the perspective of CD4, and is oriented with the viral membrane at the top of the figure and the target cell membrane at the bottom. The N- and C-termini of the truncated gp120 core are labeled, as are the positions of structures related to the gp120 variable regions, V1-V5. The L_d and L_e surface loops(12) are

shown. The position of the "Phe 43" cavity involved in CD4 binding is indicated by an asterisk. A gp120 surface implicated in binding to the CCR5 chemokine receptor (C. Rizzuto and J. Sodroski, submitted) is indicated. The perspectives in Figures 23B, C and D are indicated.

<u>Figure 34B</u>

View of the molecular surface of the gp120 outer domain, from the perspective indicated in Figure 34A. The molecular surface in the figure on the left is shaded according to the variability observed in gp120 residues among primate immunodeficiency viruses. The variability of the gp120 surface shown is underestimated since the V4 variable loop, which is not resolved in the structure, contributes to this surface. The position of the V5 region is shown. Also note the highly conserved glycosylation site (asparagine 356 and threonine/serine 358) within the L_e loop, between the V5 and V4 regions. In the figure on the right, the V4 loop and the carbohydrates are modeled, as described in Materials and Methods.

<u>Figure 34C</u>

View of the gp120 molecular surface facing the target cell. Variability is indicated in the figure on the left, using the shading scheme as in Figure 34B. Note the clear demarcation between the conserved surface, which has been implicated in the formation of CD4i epitopes(18)and in chemokine receptor binding (C. Rizzuto and J. Sodroski, unpublished observations), and the variable surface of the outer domain. The recessed binding site for CD4 is indicated, flanked by the V1/V2 stem, which is labeled. The V4 loop and the carbohydrates are modeled in the figure on the right. The figure is shaded as indicated in Figure 34B particularly carbohydrates referred to elsewhere in this report are labeled.

<u>Figure 34D</u>

View of the molecular surface of the gp120 core inner domain. In the figure on the left, variability is indicated by the shading scheme used in Figure 34B. The CD4-binding site is to the right of the figure, and the protruding V1/V2 stem is indicated. The conserved molecular surface, which is associated with the inner domain of the gp120 core, is devoid of know N-linked glycosylation. These are modeled in the figure on the right, which is shaded as described in Figure 23B.

<u>Figure 35</u>

The spatial relationship of epitopes on the HIV-1 gp120 glycoprotein.

<u>Figure 35A</u>

The molecular surface of the gp120 core is shown, from the same perspective as that in Figure 34A. The modeled N-terminal gp120 core residues, V4 loop and carbohydrate structures are included. The variability of the molecular surface is indicated, using the shading scheme described in Figure 34B. The approximate locations of the V2 and V3 variable loops are indicated. Note the well-conserved surfaces near the "Phe 43" cavity and the chemokine receptor- binding site (see Figure 34A).

<u>Figure 35B</u>

A Cα tracing of the gp120 core, oriented similarly to Figure 34A. The gp120 residues within Figure 37A of the 17b CD4i antibody are shown. The residues implicated in the binding of CD4BS antibodyies(20) are shown. Changes in these residues significantly affect the binding of at least 25 percent of the CD4BS antibodies listed in the table from the fourth series of experiments. The residues implicated in 2G12 binding(19) are shown. The V4 variable loop, which contributes to the 2G12 epitope,(19) is indicated by dotted lines (see figure 34A).

<u>Figure 35C</u>

The molecular surface of the gp120 core, oriented and shaded as in Figure 35B, is shown.

Figure 35D

Approximate locations of the faces of the gp120 core, defined by the interaction of gp120 and antibodies. The molecular surface accessible to neutralizing ligands (CD4 and CD4BS, CD4i and 2G12 antibodies) is shown in white. The neutralizing face of the complete gp120 glycoprotein includes the V2 and V3 loops, which reside adjacent to the surface shown (see Figure 35A). The approximate location of the gp120 face that is poorly accessible on the assembled envelope glycoprotein trimer and therefore elicits only non-neutralizing antibodies(5, 6) is shown. The approximate location of an immulogically "silent" face of gp120, which roughly corresponds to the highly glycosylated outer domain surface, is also shown.

Figure 36

A likely arragement of the HIV-1 gp120 glycoproteins in a trimeric complex. The gp120 core was organized into a trimeric array, based on the criteria discussed in the text. The perspective if from the target cell membrane, similar to that shown in Figure 34C. The CD4 binding pockets are indicated by black arrows, and the chemokine receptor-binding regions are darkly shaded. The lightly shaded areas indicate the more variable, glycosylated surface of the gp120 core. The approximate locations of the 2G12 epitopes are indicated by open arrows. The approximate locations for the V3 loops and V4 regions are shown. The positions of the V5 regions and some complex carbohydrate addition sites (asparaginase 276, 463, 356, 397 and 406) are shown. The approximate locations of the large V1/V2 loops, centered on the known positions of the V1/V2 stems, are indicated. On one of the gp120 subunits, the positions of the L_D and L_E loops are indicated. The distance of each of the gp120 monomers from the 3-fold symmetry axis is arbitrary.

Figures for the Fifth Series of Experiments

Figure 37

The HIV gp120 derivative used in the binding assay. The wild-type gp120 and gp41 envelope glycoproteins are shown in the upper figure. Conserved (black) and variable (white) regions (25) are indicated. The wtΔ protein, which is derived from the primary macrophage-tropic YU2 HIV-1 isolate (7), is shown beneath the wild-type envelope glycoproteins. The N-terminal and V1/V2 deletions correspond to those previously described for the HXBc2 gp120 mutants Δ82 and Δ128-194, respectively (8,9). SIG=signal peptide.

Figure 38

The gp120-CCR5 binding assay.

Figure 38A

The radiolabeled wtΔ protein was incubated either with the parental L1.2 cells or with the L1.2-CCR5 cells. Incubations were carried out either in the absence or presence of sCD4 (100nM). The wtΔ protein bound to the cells is shown. The two bands represent different glycoforms of gp120.

Figure 38B

The wtΔ protein was incubated with both sCD4 and 17b antibody at the indicated concentrations prior to adition to the L1.2-CCR5 cells. The L1.2-CCR5 cells were incubated with 2D7 anti-CCR5 antibody or MIP-1β at the indicated concentrations prior to incubation with wtΔ-sCD4 complexes. The wtΔ protein bound to the cells is shown.

Figure 38C

The amount of radiolabeled wtΔ or selected mutant envelope glycoproteins precipitated by a mixture of HIV-1-infected patient sera(Total), precipitated by sCD4 and an anti-CD4 antibody (Bound(sCD4)), or bound to L1.2-CCR5 cells (Bound(CCR5)) is shown.

Figure 39

Structure of the HIV-1 gp120 region implicated in CCR5 binding.

Figure 39A

A ribbon drawing of the HIV-1 gp120 glycoprotein (6) complexed with CD4 is shown. The perspective is that from the target cell membrane. The two amino-terminal domains of CD4 are shown. The gp120 inner domain is shown, the outer domain is shown and the "bridging sheet" is shown. The gp120 residues in which changes resulted in a ≥90% decrease in CCR5 binding are labeled. The V1/V2 stem and base of the V3 loop (strands β12 and β13 and the associated turn) are indicated.

Figure 39B

A molecular surface of the gp120 glycoprotein from the same perspective as that of Figure 39A is shown. Shaded surfaces are associated with gp120 residues in which changes resulted in either a ≥ 75% decrease, a ≥ 90% decrease or a ≥ 50% increase in CCR5 binding, when CD4 binding was at least 50% of that seen for the wtΔ protein.

Figure 39C

The surface depicted in Figure 39B is shaded according to the degree of conservation observed among primate immunodeficiency viruses (25).

Figure 39D

The molecular surface of the gp120 glycoprotein is shown, indicating residues in which changes resulted in a ≥ 70% decease in 17b antibody binding, in the absence of sCD4.

Figure 39E

The molecular surface of the gp120 glycoprotein is shown, indicating residues in which changes resulted in a ≥ 70% decrease in CG10 antibody binding in the presence of sCD4. Residues in which changes significantly decreased CD4 binding (and thus indirectly decreased CG10 binding) are not shown. Images were made with Midas-Plus (Computer Graphics Lab, University of California, San Francisco) and GRASP (26).

Mimcs of CD4 With Enhanced Affinity For gp120

Figure 40

Illustration of the gp120-binding domain of CD4 and its interaction with the hydrophobic pocket of gp120.

Figure 41A

Active Halogen Reaction Scheme for modifying cysteine 43 mutants of CD4.

Figure 41B

Pyridyl Disulfide Reaction Scheme for modifying cysteine 43 mutants of CD4.

Figure 42

Some specific examples of cysteine 43 mutant derivatives produced with the active halogen reaction scheme.

Figure 43A

General reaction scheme for using a bifunctional reagent to modify the gp120-binding domain of CD4.

Figure 43B

Reaction scheme for using a bifunctional reagent to modify a residue in the gp120-binding domain of CD4 as applied to a cysteine residue.

Figure 44A and B

Use of 3-(2-pyridyldithio)propionic acid N-hydroxysuccinimide ester (SPDP), a bifunctional reagent, as an adaptor for modifying a residue in the gp120-binding domain of CD4.

Figure 45

Illustration of how modification can improve the fit between the gp120-binding domain of CD4 and the hydrophobic pocket in gp120.

Figure 46

Illustration of some of the residues lining the hydrophobic pocket of gp120. The residues lining the hydrophobic pocket of gp120 include: Trp (112), Leu (116), Pro (118), Phe (210), Val (255), Ser (375), Asn (377), Phe (382), Ile (424), Met(426), Trp (427), Asn (428), Ala (433), Gly (473), and Met (475)

Figure 47

Computer-generated ribbon drawing of the tertiary structure of CD4 and gp120 interacting. CD4 is toward the bottom and gp120 is toward the top.

Figure 48

Reaction scheme for chemically modifying tyrosine residues. R1 may be selected from the group shown in Figure 44. An alterative mechanism may be achieved as shown on page 365 of Structure and Protein Chemistry by Jack Kyte (1994), in which a diazonium salt participate in electrophilic aromatic substitution with tyrosine.

Figure 49

Schematic showing the structural domains of gp120.

gp120 Variants as Vaccine For HIV Infection

Figure 50

Depiction of the gp120 Oligomer.

Figure 51

Depiction of the pocket of gp120 formed after the binding of CD4 to gp120.

Figure 52

The topology for the gp120 (Δ82, ΔV1/2, ΔV3, ΔC5) construct.

Coordinates and Contacts

Figure 53

Shows the x-ray crystallography obtained atomic coordinate data of the gp120 ternary complex of HIV-1 GP120 complexed with CD4 and Fab 17b having space group P2221 and unit cell dimensions a=71.643, b=88.130, c=196.7. The raw data and the coordinates were described in U.S. Serial No. 09/100,764, filed June 18, 1998 and U.S. Serial No. 08/967,708, filed November 10, 1997, on which this subject application claims priority. These documents are subjected for public inspection. The contents of these applications are incorporated into this application by reference. The coordinates have been deposited in the in the Brookhaven Protein Data

Bank with the accession code Igcl. In addition, the coordinates may be obtained in the worldwide web: www.pbd.bnl.gov after inputting "Igcl" for the above coordinates.

Figure 54

Provides a detailed list of all the contacts between gp120 (designated here as molecule A) and CD4 (designated here as molecule B).

Figure 55

Provides a detailed list of all the contacts between gp120 (designated here as molecule A) and the Fab 17b (the light chain is designated here as molecule C; the heavy chain is designated here as molecule D).

Detailed Description of the Invention

The invention relates to a crystals of gp120 suitable for x-ray diffraction. The three dimensional structure of gp120 provides information which has a number of uses; principally related to the development of pharmaceutical compositions which mimic the action of gp120. In an embodiment, the crystals comprising a portion of gp120. The portion of gp120 may contain the CD4 binding site. In another embodiment, the portion contains the chemokine receptor binding site. In a further embodiment, the portion of gp120 contains both the CD4 binding site and the chemokine receptor binding site.

In a separate embodiment, the portion of gp120 will be at least 100 amino acids long. In a preferred embodiment, the portion is at least 200 amino acid long.

The essence of the invention resides in the obtaining of crystals of gp120 of sufficient quality to determine the three dimensional (tertiary) structure of the protein by x-ray diffraction methods.

This invention provides crystals of sufficient quality to obtain a determination of the three-dimensional structure of gp120 to high resolution, preferably to the resolution of 2.5 angstroms.

The value of crystals of gp120 extends beyond merely being able to obtain a structure for gp120. The knowledge of the structure of gp120 provides a means of investigating the mechanism of action of these proteins in the body. For example, binding of these proteins to various receptor molecules can be predicted by various computer models. Upon discovering that such binding in fact takes place, knowledge of the protein structure then allows chemists to design and attempt to synthesize

molecules which mimic the binding of gp120 to its receptors. This is the method of "rational" drug design.

One skilled in the art may use one of several methods to screen chemical entities for their ability to associate with gp120. This process may begin by visual inspection of, for example, the active site on the computer screen based on the gp120 coordinates. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

GRID [P.J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem. 28:849-857 (1985)]. GRID is available from Oxford Universit, Oxford, UK.

MCSS [A. Miranker and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method", Proteins: Structure, Function and Genetics, 11:29-34 (1991)]. MCSS is available from Molecular Systems, Burlington, MA.

AUTODOCK [D.S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins, Structure, Function, and Genetics, 195-202 (1990)] AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

Once suitable entities or fragments have been selected,

they can be assembled into a single compound or inhibitor. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of gp120. This would be followed by manual model building using software as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

CAVEAT [P.A. Bartell et al., "CAVEAT: A Program of Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.

3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35:2145-2154 (1992).

Instead of proceeding to build a gp120 inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other type of binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include:

LUDI [H.-J. Bohm "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6:61-78 (1992)]. LUDI is available from Biosym Technologies, San Diego, CA.

LEGEND [Y. Nishibata and A. Itai, Tetrahedron, 47:8985 (1991)]. LENGEND is available from Molecular Simulations, Burlington, MA.

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N.C. Cohen et al, "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33:883-894 (1990). See also, M.A. Navia and M.A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2:202-210 (1992). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, e.g., P.S. Farmer, Drug Design, Ariens, E.J., ed., Vol. 10, pp. 119-143 (Academic Press, New York 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; C. Verlinde, Structure, 2:577-587 (1994); and I.D. Kuntz, Science 257:1078-1082 (1992). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Thus, using these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds is effectively eliminated.

Once identified by the modeling techniques, the gp120 or CD4 antagonist may be tested for bioactivity using standard techniques. For example, structure of the invention may be used in binding assays using conventional formats to screen inhibitors. Suitable assays for use herein include, but are not limited to, the enzyme-linked immunosorben assay (ELISA), or a

fluoresence quench assay. Other assay formats may be used; these assay formats are not a limitation on the present invention.

In another aspect, the gp120 structure of the invention permit the design and identification of synthetic compounds and/or other molecules which have a shape complimentary to the conformation of the gp120 active site of the invention. Using known computer systems, the coordinates of the gp120 structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the invention. Subsequently, suitable candidates identified as above may be screened for the desired gp120 inhibitory bioactivity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block gp120 activity.

Accordingly, this invention also provides material which is the basis for the rational design of drugs which mimic the action of gp120.

The subject invention provides a crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120.

The subject invention also provides the above-described crystals, which effectively diffract X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 4 angstroms or better than 4 angstroms.

The subject invention also provides the above-described

crystals, which effectively diffract X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 2.5 angstroms or better than 2.5 angstroms.

The subject invention also provides the above-described crystals, wherein the portion of gp120 comprises a CD4 binding site.

The subject invention further provides the above-described crystals, further comprising a compound bound to the CD4 site.

The subject invention also provides the above-described crystals, wherein the portion of gp120 comprises a chemokine receptor binding site.

The subject invention also provides the above-described crystals, further comprising a compound bound to the chemokine receptor binding site.

The subject invention also provides the above-described crystals, wherein the portion of gp120 comprises a CD4 binding site and a chemokine receptor binding site.

The subject invention also provides the above-described crystals, further comprising of a first compound bound to the CD4 binding site of the polypeptide and a second compound bound to the chemokine receptor binding site of the polypeptide.

The subject invention also provides the above-described crystals, wherein the first compound is the second compound.

The subject invention also provides the above-described crystals, wherein the crystal is arranged in a space

group $P222_1$, so as to form a unit cell of dimensions a=71.6 Å, b= 88.1 Å, c=196.7 Å, and which effectively diffracts x-rays for determination of the atomic coordinates of the gp120 to a resolution of 2.5 Å or better.

The subject invention also provides the above-described crystals, wherein the polypeptide is a variant of gp120 lacking the V1, V2, V3, and C5 regions.

The subject invention also provides the above-described crystals, wherein the gp120 variant comprises a portion of the conserved stem of the V1/V2 stem-loop structure.

The subject invention also provides the above-described crystals, wherein the gp120 variant comprises a portion of the base of the V3 loop.

The subject invention also provides the above-described crystals, wherein the gp120 variant comprises a portion of the C5 region.

The subject invention also provides the above-described crystals, wherein the polypeptide is a variant of gp120 with 5% by weight of the carbohydrate residues linked to the gp120 in substantially the same manner as they are linked to gp120 in unmodified gp120.

The subject invention also provides the above-described crystals, wherein the polypeptide is a variant of gp120 with 15% by weight of the carbohydrate residues linked to the gp120 polypeptide in substantially the same manner as they are linked to gp120 in unmodified gp120.

The subject invention also provides the above-described crystals, further comprising a Fab, a CD4, a polypeptide having amino acid sequence of a portion of CD4, or a

combination thereof, bound to the gp120.

The subject invention also provides the above-described crystals, wherein the Fab is produced from an antibody to a discontinuous epitope.

The subject invention also provides the above-described crystals, wherein the monoclonal antibody is designated 17b.

The subject invention additionally provides a method for producing a crystal suitable for X-ray diffraction comprising: (a) deglycosylating a polypeptide having amino acid sequence of a portion of a gp120 wherein said portion is produced by deleting or replacing part of the gp120 to reduce the surface loop flexibility; (b) contacting the polypeptide with a ligand so as to form a complex which exhibits restricted conformational mobility; and (c) obtaining crystal from the complex so formed to produce a crystal suitable for X-ray diffraction.

The subject invention also provides the above-described methods, wherein the V1, V2, or V3 loop of the gp120 contained in the polypeptide are partially truncated, deleted or replaced.

The subject invention also provides the above-described methods, wherein the polypeptide lacks the V1, V2, V3 and C5 loop of the gp120.

The subject invention also provides the above-described methods, wherein the polypeptide also lacks up to fifty N-terminal amino acids of the gp120 or up to fifty C-terminal amino acid of gp120.

The subject invention also provides the above-described

methods, wherein the ligand is a Fab, a CD4, or a polypeptide having amino acid sequence of a portion of CD4.

The subject invention also provides the above-described methods, wherein the resulting polypeptide after the deglycosylation contains at least 5% of the carbohydrate.

The subject invention also provides the crystal produced by the above-described methods.

The subject invention also provides a method for identifying a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and (b) determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the gp120.

The subject invention also provides a method for designing a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and (b) designing a compound to fit the binding site.

Structure-based drug design has been known and was previously described. See e.g., Bugg et al. (1993) Sci. Amer., December: 92-98; Giranda (1994) Structure, 2:695-698; Lam et al. (1994) Science 263:380-384; and Navia et al. (1994) Circulation **89(4)**:1557-1566.

The subject invention also provides the above-described methods, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

The subject invention also provides the above-described methods, wherein the atomic coordinates are set forth in Figure 53.

The subject invention also provides a pharmaceutical composition comprising the compound identified by the above-described methods and a pharmaceutically acceptable carrier.

For the purposes of this invention "pharmaceutically acceptable carriers" means any of the standard pharmaceutical carriers. Examples of suitable carriers are well known in the art and may include, but not limited to, any of the standard pharmaceutical carriers such as a phosphate buffered saline solutions, phosphate buffered saline containing Polysorb 80, water, emulsions such as oil/water emulsion, and various type of wetting agents. Other carriers may also include sterile solutions, tablets, coated tablets, and capsules.

Typically such carriers contain excipients such as starch, milk, sugar, certain types of clay, gelatin, stearic acid or salts thereof, magnesium or calcium sterate, talc, vegetable fats or oils, gums, glycols, or other known excipients. Such carriers may also include flavor and color additives or other ingredients. Compositions comprising such carriers are formulated by well known conventional methods.

The subject invention also provides the above-described methods, wherein the compound is not previously known.

The subject invention also provides the compounds

identified by the above-described methods.

The subject invention also provides the compound designed by the above-described methods.

The subject invention also provides a composition comprising the above-described compounds and a suitable carrier.

This invention also provides a method of inhibiting the interaction of HIV-gp120 with CD4 which comprises administering to a mammal a compound, with the proviso that the compound is not CD4, capable of disrupting two or more of the contacts between gp120 and CD4 as set forth in Figure 54.

This invention also provides a method for identifying a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and (b) determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the CD4 binding site of the gp120.

The molecular interaction on HIV with CD4 is between the HIV envelope glycoprotein gp120 and the D1 domain of CD4. The crystal structure of the complex between the deglycosylated core of gp120 and the D1D2 fragment of human CD4 defines this interaction in atomic detail (*Nature* paper). Although there is an extensive interface between these components, the nexus of the interaction brings together those residues demonstrated by mutational analyses to those most crucial for

binding. Phe 43 and Arg 59 from CD4 and Asp 368, Glu 370 and Trp 427 from gp120 (*Nature* paper, Fig. 3j). This dominant sub-site comprises gp120 residues 365-368, 370-371, 425-430 and 473. In addition, Phe 43 closes off a pocket on the HIV surface to form a large cavity (152Å^3) at this interface (*Nature* paper, Fig. 3b). Residues that line the Phe 43 pocket include Trp 112, Val 255, Thr 257, Glu 370, Phe 382, Tyr 384, Try 427, Met 475 and main-chain atoms of 256 and 375-377.

The atomic coordinates of the crystallographic model also define the binding surface to be exploited by high-affinity compounds that will have the property to inhibit the gp120-CD4 interaction, and thereby the attachment of HIV to CD4-positive cells. This definition of the surface provides practioners skilled in the art with the means to design such compounds. Appropriate fragments or chemicals entities for the design of such compounds can be formed through the use of specialized computer programs such as GRID, DOCK and LUDI. Computer graphical representatives of these entitles can then be composed into appropriate chemical compounds, using the crystal structure as a template. Medicinal chemists skilled in the art can then synthesize appropriate chemical compounds to implement these designs. Not all such compounds will bind and have inhibitory properties, but a sufficient portion will do so to provide the designed lead compounds for drug discovery. Such leads can then be developed by the methods of structure-based drug design using crystallized complexes between these compounds and deglycosylated core gp120.

A compound that will bind to the dominant sub-site of the CD4 intermolecular interface will have surface properties that are complementary to the surface properties of the sub-site itself. The surface of the

sub-site can be characterized by the GRASP computer program with respect to curvature, electrostatic potential, and hydrophobicity. The complementary surface to this one (i.e., convex vs. concave, positive vs. negative, etc.) Defines an envelope that will correspond to the binding portion of the molecular surface of an inhibitory compound. Thus, any compound that has an accessible conformation such as to match the surface that is complementary to the HIV gp120 binding surface is one that has a high probability for inhibitory binding. Since it should be possible for skilled practitioners to design and synthesize such compounds when instructed by the template of the HIV gp120 structure and the CD4 binding elements, these compounds defined by congruence with the complementary surface can be considered inventions by the process hereby defined.

This invention also provides a method for designing a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and (b) designing a compound to fit the CD4 binding site.

This invention also provides the above-described methods, wherein the crystal further comprising a CD4, a second polypeptide having amino acid sequence of a portion of CD4, or a compound known to be able to bind to the CD4 site of the gp120, bound to the polypeptide.

This invention also provides the above-described methods, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

This invention also provides the above-described methods, wherein the atomic coordinates are set forth in Figure 53.

This invention also provides a pharmaceutical composition comprising the compound identified the by above-described methods and a pharmaceutically acceptable carrier.

This invention also provides the above-described methods, wherein the compound is not previously known.

This invention also provides the compound identified by the above-described methods.

This invention also provides the compound designed by the above-described methods.

This invention also provides a composition comprising the above-described compounds and a suitable carrier.

This invention also provides a method of inhibiting Human Immunodeficiency Virus infection in a subject comprising adminstering effective of amount of the above-described composition to the subject.

In embodiments of the above-described methods, the above-described compounds are nonpeptidyl.

This invention provides a method for identifying a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of

binding to the chemokine receptor; and (b) determining whether a compound would fit into the binding site, a positive fit indicating that the compound is capable of binding to the chemokine receptor binding site of the gp120.

This invention also provides a method for designing a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and (b) designing a compound to fit the chemokine receptor binding site.

This invention also provides the above-described methods, wherein the crystal further comprises a chemokine receptor, a second polypeptide having amino acid sequence of a portion of chemokine receptor, an antibody or a Fab capable of binding to the chemokine receptor binding site or a compound known to be capable of binding to the chemokine receptor binding site, bound to the polypeptide.

This invention also provides the above-described methods, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

This invention also provides the above-described methods, wherein the atomic coordinates are set forth in Figure 53.

The pharmaceutical composition comprising the compound identified by the above-described methods and a pharmaceutically acceptable carrier.

This invention also provides the above-described methods, wherein the compound is not previously known.

This invention provides compounds identified by the above-described methods. This invention provides compounds designed by above-described methods.

A composition comprising the above-described compounds and a suitable carrier.

Additionally, this invention provides a method of inhibiting Human Immunodeficiency Virus infection in a subject comprising adminstering effective of amount of the above-described composition to the subject, thereby inhibiting Human Immunodeficiency Virus infection.

This invention further provides a method of inhibiting the interaction of HIV-gp120 with chemokine receptor which comprises administering to a mammal a compound capable of disrupting two or more of the contacts between gp120 and chemokine receptor as set forth in Figure 55, thereby inhibiting the interaction of HIV-gp120 with chemokine receptor with the proviso that the compound is not a chemokine receptor. In an embodiment, the compound is nonpeptidyl.

Table Summarizing the CCR5-binding residues of gp120

SET A	117, 121, or 123
SET B	207
SET C	330
SET D	419, 420, 421, 422, 437, 438, 440, 441, 442, or 444

This invention further provides a method of inhibiting cell entry by HIV, comprising blocking or inhibiting the residues from 2 or more the sets of the CCR5-binding residues set forth above, thereby inhibiting or preventing gp120 from binding to CCR5 and thereby

inhibiting cell entry by HIV.

This invention also provides the above described method wherein 3 or more the sets of the CCR5-binding residues set forth above are blocked or inhibited from interacting with CCR5.

This invention also provides the above described methods, wherein the blocking or inhibiting comprises contacting the CCR5-binding residues with an antibody.

This invention also provides the above-described methods, wherein the compound is nonpeptidyl.

This invention provides a substance mimicking the human immunodeficiency virus envelope glycoprotein gp120-binding region of CD4 wherein the size of a residue or analog thereof, corresponding to the phenylalanine at position 43 in the native CD4, is larger than the size of phenylalanine so as to fill the pocket on gp120 which extends beyond position 43 in the gp120/CD4 complex and increase the affinity for gp120.

As used herein, residue or analog thereof includes amino acids (both individually and as part of a polypeptide chain), modified amino acids, amino acid analogs, and chemical compounds that can be substituted for the amino acids that ordinarily make up the CD4 polypeptide chain. (Also see the discusion of peptidomimetics, synthetic polypeptides, and polypeptide analogs below.)

This invention also provides the above-described substance, wherein the substance is a peptidomimetic analog, a synthetic polypeptide, a standard polypeptide, or a polypeptide analog.

As used herein, the substance mimicking the gp120-

binding domain of CD4 embraces a wide range of compounds. In addition to naturally-occurring forms of polypeptides derived from CD4, the present invention also embraces other CD4 polypeptides such as polypeptide analogs of CD4. Such analogs include fragments of CD4. Following the procedures of the published application by Alton et al. (WO 83/04053), one can readily design and manufacture genes coding for microbial expression of polypeptides having primary conformations which differ from that herein specified for in terms of the identity or location of one or more residues (e.g., substitutions, terminal and intermediate additions and deletions). Alternately, modifications of cDNA and genomic genes can be readily accomplished by well-known site-directed mutagenesis techniques and employed to generate analogs and derivatives of the CD4 polypeptide. Such products share at least one of the biological properties of CD4 but may differ in others.

As examples, products of the invention include those which are foreshortened by e.g., deletions; or those which are more stable to hydrolysis (and, therefore, may have more pronounced or longerlasting effects than naturally-occurring products); or which have been altered to delete or to add one or more potential sites for O-glycosylation and/or N-glycosylation or which have one or more cysteine residues deleted or replaced by e.g., alanine or serine residues and are potentially more easily isolated in active form from microbial systems; or which have one or more tyrosine residues replaced by phenylalanine and bind more or less readily to target proteins or to receptors on target cells. Also comprehended are polypeptide fragments duplicating only a part of the continuous amino acid sequence or secondary conformations within gp120, which fragments may possess one property of gp120 and not others. It is noteworthy that activity is not necessary for any one or

more of the polypeptides of the invention to have therapeutic utility or utility in other contexts, such as in assays of gp120 antagonism. Competitive antagonists may be quite useful in, for example, cases of overproduction of gp120.

Of applicability to polypeptide analogs of the invention are reports of the immunological property of synthetic peptides which substantially duplicate the amino acid sequence extant in naturally-occurring proteins, glycoproteins and nucleoproteins. More specifically, relatively low molecular weight polypeptides have been shown to participate in immune reactions which are similar in duration and extent to the immune reactions of physiologically-significant proteins such as viral antigens, polypeptide hormones, and the like. Included among the immune reactions of such polypeptides is the provocation of the formation of specific antibodies in immunologically-active animals [Lerner et al., Cell, 23, 309-310 (1981); Ross et al., Nature, 294, 654-658 (1981); Walter et al., Proc. Natl. Acad. Sci. USA ,78, 4882-4886 (1981); Wong et al., Proc. Natl. Sci. USA, 79, 5322-5326 (1982); Baron et al., Cell, 28, 395-404 (1982); Dressman et al., Nature, 295, 185-160 (1982); and Lerner, Scientific American, 248, 66-74 (1983). See also, Kaiser et al. [Science, 223, 249-255 (1984)] relating to biological and immunological properties of synthetic peptides which approximately share secondary structures of peptide hormones but may not share their primary structural conformation.

This invention also provides the above-described substances, wherein the modification increases the hydrophobicity or size of the residue or analog thereof at position 43.

This invention also provides the above-described

substances, wherein the modification comprises directly or indirectly linking a hydrophobic compound to a residue or analog thereof at position 43 of the domain.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that is bulkier than phenylalanine.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 7 Å across its longest dimension.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 10 Å across its longest dimension.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 15 Å across its longest dimension.

This invention provides the above described substance which enhances hydrophobic interactions to residues that line the pocket. In another embodiment, this invention provides the above described substance which enhances hydrogen bonding to residues that line the pocket. In a separate embodiment, this invention provides the above described substance which enhances electrostatic interactions with residues that line the pocket. In a still separate embodiment, this invention provides the above described substance which enhances surface fit with residues that line the pocket.

This invention also provides the above-described

substances, wherein the modification involves replacemnet of the residue at position 43 with a cysteine. This invention further provides that the substition of the sulfhydryl group of this cysteine.

This invention also provides the above-described substances, wherein the modification involves replacement of the residue at position 43 with a tyrosine. This invention further provides that the substition of this tyrosine

This invention also provides the above-described substances, wherein the modification comprises directly or indirectly linking an adaptor residue or analog thereof to position 43.

This invention also provides the above-described substances, wherein the adaptor residue or analog thereof is directly or indirectly linked to a hydrophobic compound, thus forming a complex.

This invention also provides the above-described substances, wherein the complex is bulkier than phenylalanine.

This invention also provides the above-described substances, wherein the complex is larger than 7 Å across its longest dimension.

This invention also provides the above-described substances, wherein the complex's longest dimension is longer than phenylalanine's longest dimension

This invention also provides the above-described substances, wherein the complex is larger than 10 Å across its longest dimension.

substances, wherein the modification results in a residue or analog thereof, wherein the residue's longest dimension is longer than phenylalanine's longest dimension.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that contains a localization of negative charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that contains a localization of charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that contains at least one additional hydroxyl group.

Placing a tyrosine residue at position 43 is an example of a modification resulting in a residue that contains a hydroxyl group. Further, the oxygen of the hydroxyl group has a localization of negative charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120. Further, the hydrogen of the hydroxyl group has a localization of charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

This invention also provides the above-described

This invention further provides a pharmaceutical composition capable of inhibiting cell entry by HIV, comprising (a) an effective amount of the above-described substance; and (b) a pharmaceutically acceptable carrier.

The actual effective amount will be based upon the size of the polypeptide, the biodegradability of the polypeptide, the bioactivity of the polypeptide and the bioavailability of the polypeptide. If the polypeptide does not degrade quickly, is bioavailable and highly active, a smaller amount will be required to be effective. The effective amount will be known to one of skill in the art; it will also be dependent upon the form of the polypeptide, the size of the polypeptide and the bioactivity of the polypeptide. Variants of CD4 with lower affinity for gp120 will require higher dosages than variants of CD4 with higher affinity for gp120. One of skill in the art could routinely perform empirical activity tests to determine the bioactivity in bioassays and thus determine the effective amount.

Pharmaceutically acceptable carriers are well known to those skilled in the art and have been described supra.

A pharmaceutical composition for treating or preventing HIV infection, comprising (a) an effective amount of the above-described substances; and (b) a pharmaceutically acceptable carrier.

This invention further provides a composition capable of inhibiting cell entry by HIV, comprising (a) an effective amount of the above-described substances; and (b) a suitable carrier.

This invention further provides a pharmaceutical composition for treating or preventing HIV infection,

comprising (a) an effective amount of the above-described substances; and (b) a pharmaceutically acceptable carrier.

This invention further provides a composition for treating or preventing HIV infection, comprising (a) an effective amount of the above-described substances; and (b) a suitable carrier.

This invention further provides a method of inhibiting cell entry by HIV, comprising contacting the cells with an effective amount of the above-described substances, thereby inhibiting cell entry by HIV.

This invention further provides a method of treating or preventing HIV infection in a subject, comprising administering to the subject an effective amount of the above-described substances, thereby treating or preventing HIV infection.

The invention provides a variant of gp120 which presents a hidden, conserved, neutralization epitope. In an embodiment, the amino acid of the above variant at position 375 is changed from a Serine to a Trptophan. In a further embodiment, the variant further comprise one of the following changes: 88N to P, 102E to L, 113D to R, 117K to W, 257T to A, 266A to E, 386N to Q, 395W to S, 421K to L, 470P to G, 475M to S, 485K to V or a combination thereof.

This invention further provides a composition comprising the above-described variant and a suitable carrier.

In a specific embodiment, "composition" as used herein means pharmaceutical compositions comprising therapeutically effective amounts of polypeptide

products of the invention together with suitable diluents, preservatives, solubilizers, emulsifiers, adjuvants and/or carriers useful in therapy. A "therapeutically effective amount" as used herein refers to that amount which provides a therapeutic effect for a given condition and administration regimen. Such compositions are liquids or lyophilized or otherwise dried formulations and include diluents of various buffer content (e.g., Tris-HCl., acetate, phosphate), pH and ionic strength, additives such as albumin or gelatin to prevent absorption to surfaces, detergents (e.g., Tween 20, Tween 80, Pluronic F68, bile acid salts). solubilizing agents (e.g., glycerol, polyethylene glycerol), anti-oxidants (e.g., ascorbic acid, sodium metabisulfite), preservatives (e.g., Thimerosal, benzyl alcohol, parabens), bulking substances or tonicity modifiers (e.g., lactose, mannitol), covalent attachment of polymers such as polyethylene glycol to the protein, complexation with metal ions, or incorporation of the material into or onto particulate preparations of polymeric compounds such as polylactic acid, polglycolic acid, hydrogels, etc, or onto liposomes, microemulsions, micelles, unilamellar or multilamellar vesicles, erythrocyte ghosts, or spheroplasts. Such compositions will influence the physical state, solubility, stability, rate of in vivo release, and rate of in vivo clearance of the admininstered materials. The choice of compositions will depend on the physical and chemical properties of the protein having the biological activity. For example, a product derived from a membrane-bound form of the protein may require a formulation containing detergent. Controlled or sustained release compositions include formulation in lipophilic depots (e.g., fatty acids, waxes, oils). Also comprehended by the invention are particulate compositions coated with polymers (e.g., poloxamers or poloxamines) and the variants coupled to antibodies

directed against tissue-specific receptors, ligands or antigens or coupled to ligands of tissue-specific receptors. Other embodiments of the compositions of the invention incorporate particulate forms protective coatings, protease inhibitors or permeation enhancers for various routes of administration, including parenteral, pulmonary, nasal and oral.

For the purposes of this invention "suitable carriers" means any of the standard carriers used in the pharmaceutical industry. Examples of suitable carriers are well known in the art and may include, but not limited to, any of the standard pharmaceutical carriers such as a phosphate buffered saline solutions, phosphate buffered saline containing Polysorb 80, water, emulsions such as oil/water emulsion, and various type of wetting agents. Other carriers may also include sterile solutions, tablets, coated tablets, and capsules.

Typically such carriers contain excipients such as starch, milk, sugar, certain types of clay, gelatin, stearic acid or salts thereof, magnesium or calcium sterate, talc, vegetable fats or oils, gums, glycols, or other known excipients. Such carriers may also include flavor and color additives or other ingredients. Compositions comprising such carriers are formulated by well known conventional methods.

This invention also provides a vaccine comprising the above-described variant. Such a vaccine may further comprise a suitable adjuvant.

Vaccines and adjuvants are well-known to those skilled in the art. Using a vaccine, comprising adjuvants or not, one may induce or stimulate the immune response of an individual. The immune response may vary, e.g. a humoral or cell-mediated immune response. Adjuvants are

chemical compounds that enhance the immunogenicity of the vaccine so as to enhance the stimulation and induction of the immune response.

In a specific embodiment, the vaccine is administered to a subject. As used herein, "subject" means any animal or artificially modified animal capable of becoming HIV-infected. Artificially modified animals include, but are not limited to, SCID mice with human immune systems.

In the preferred embodiment, the subject is a human. In another embodiment, the subject is a human infected with HIV.

As used herein, a "human infected with HIV" means an individual having at least one of his own cells infected by HIV. As used herein, an HIV-infected cell is a cell wherein HIV has been produced. A non-HIV-infected subject means a subject not having any cells infected by HIV. In one embodiment, a non-HIV-infected subject is an HIV-exposed subject. As used herein, an HIV-exposed subject is a subject who has HIV present in his body, but has not yet become HIV-infected. For example, a subject may become HIV-exposed upon receiving a needle stick injury with an HIV-contaminated needle.

In a specific embodiment of the invention, one may first crystals of gp120 of sufficient quality to determine the three dimensional (tertiary) structure of the protein by x-ray diffraction methods. The value of crystals of gp120 extends beyond merely being able to obtain a structure for gp120. The knowledge of the structure of gp120 provides a means of investigating the mechanism of action of these proteins in the body. For example, binding of these proteins to various receptor molecules can be predicted by various computer models. Upon discovering that such binding in fact takes place,

knowledge of the protein structure then allows chemists to design and attempt to synthesize molecules which mimic the binding of gp120 to its receptors. This is the method of "rational" drug design. Using such methods, one may determine a variant of gp120 which presents a hidden, conserved, neutralization epitope.

This invention further provides an antibody induced by the above-described vaccine. Specifically, the antibody may be a polyclonal antibody or a monoclonal antibody.

An antibody comprises intact immunoglobulin molecules, substantially intact immunoglobulin molecules and those portions of an immunoglobulin molecule that contains the paratope, including those portions known in the art as Fab, Fab', $F(ab')_2$ and F(v), which portions are preferred for use in the therapeutic methods described herein. In another embodiment, the antibody is a single-chain antibody.

As used herein, "polyclonal antibodies" may comprise different sera whereas "monoclonal antibody" comprises antibodies, each of which will reconize one single epitope. Methods for production of monoclonal antibodies are well-known in the art.

In order to determine variants of gp120 which presents a hidden, conserved, neutralization epitope, the gp120 structure of the invention permit the design and identification of synthetic compounds and/or other molecules which have a shape complimentary to the conformation of the gp120 active site of the invention. Using known computer systems, the coordinates of the gp120 structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the invention. Subsequently, suitable

[redacted]

candidates identified as above may be screened for the desired gp120 inhibitory bioactivity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block gp120 activity. Such compounds may prove useful as vaccines.

This invention provides a vaccine comprising a polypeptide having 6 or more amino acids in the same spatial proximity to each other as the amino acids from the Phe 43 cavity of naturally occurring gp120.

This invention also provides the above-described vaccine, wherein the 6 or more amino acids are identical to the amino acids of naturally occurring gp120.

This invention further provides the above-described vaccines, wherein the amino acids are within 1 angstrom of their distances in naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the amino acids are within 3 angstroms of their distances in naturally occurring gp120.

This invention provides the above-described vaccines, wherein the amino acids are within 5 angstroms of their distances in naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the polypeptide is or is part of a conserved neutralization epitope.

This invention further provides the above-described vaccines, further comprising a carrier.

This invention also provides the above-described

vaccines, further comprising an adjuvant.

This invention provides a vaccine comprising a polypeptide having 6 or more continuous amino acids from the Phe 43 cavity of gp120.

This invention provides the above-described vaccines, wherein the polypeptide is or is part of an epitope a conserved neutralization epitope.

This invention also provides the above-described vaccines, further comprising a carrier.

This invention further provides the above-described vaccines, further comprising an adjuvant.

This invention further provides a vaccine comprising a polypeptide having 6 or more amino acids in the same spatial proximity to each other as the surface accessible amino acids adjacent to the Phe 43 cavity of naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the 6 or more amino acids are identical to the amino acids of naturally occurring gp120.

This invention provides the above-described vaccines, wherein the amino acids are within 1 angstrom of their distances in naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the amino acids are within 3 angstroms of their distances in naturally occurring gp120.

This invention further provides the above-described vaccines, wherein the amino acids are within 5 angstroms

of their distances in naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the polypeptide is or is part of a conserved neutralization epitope.

This invention further provides the above-described vaccines, further comprising a carrier.

This invention also provides the above-described vaccines, further comprising an adjuvant.

This invention also provides the above-described vaccines, wherein the surface accessible amino acids comprise Lysine 432, Proline 369, and Threonine 373.

This invention further provides a vaccine comprising a polypeptide having 6 or more continuous surface accessible amino acids adjacent to the Phe 43 cavity of gp120.

This invention also provides the above-described vaccines, wherein the polypeptide is or is part of a conserved neutralization epitope.

This invention further provides the above-described vaccines, further comprising a carrier. This invention also provides the above-described vaccines, further comprising an adjuvant.

Many animal viruses target specific host cells for infection by attachment to cell surface receptor molecules unique to these cells. These viral receptors have particular roles in the normal functioning of these cells. The virus simply subverts these functions in order to effect entry into the cell. Certain molecules on the viral surface can in turn be the target of

antibodies raised by the host in defense against this parasitic attack. Viruses can evade such antibody immunity by mutating their surface proteins. The receptor binding site, however, must remain constant. It therefore evolves to be protected from antibody surveillance.

Application to HIV vaccine:

The viral surface protein, gp120 (which appears to be a trimer on the surface of the virion), plays a central role in immune evasion. The precise mechanism of gp120 immune evasion thus far remains unknown, but the structure of the gp120 - CD4 - Fab 17b complex reveals several crucial features:

1. The CD4 binding site is very large (larger than the typical antibody footprint).
2. The V1/2 variable loop is oriented to mask the CD4 binding site.
3. The V3 variable loop is not near the CD4 binding site (on a monomer), but the tip of this loop could interact with Fab 17b, which marks the second receptor binding site.
4. The CD4 binding site undergoes conformational changes upon CD4 binding.

From the structure, the following details of the mechanism of gp120 immune evasion become clear:

1. The V1/2 loop occludes the CD4 binding site and allow CD4 binding. With most viruses, which bind to rare cellular receptors, such a mechanism of immune evasion would not work; the virus would not find the proper receptor at high enough frequency to ensure viral propagation. It is the clustering of CD4 positive cells in such places as the thymus which allows this mechanism to function in the particular case of HIV.

2. The virus masks constant regions involved in both CD4 and second receptor binding; the act of CD4 binding induces conformational changes in gp120 which unmask these regions.
3. The V3 loop, which forms part of the conserved second receptor binding site, is one of the regions unmasked by CD4 binding.

This invention uses an antigen which mimics the conformation of gp120 on the surface of the HIV-virion, with deletions in the variable loop regions to expose the conserved CD4 binding site. It is already known that CD4-binding site antibodies are widely neutralizing, and moreover, are found in virtually all patients (although they tend to only be found late in the course of infection -- the initial antibodies produced early in the course of infection have the V1/2 or V3 loop as epitopes).

This invention provides a vaccine composed of a stabilized oligomer of gp120, with truncations in the variable loop regions to expose the conserved CD4 binding site, would elicit widely neutralizing antibodies against HIV.

Details: Oligomer stabilization (Figure 50):

1. Appropriately placed cysteine mutations, which would then form stabilizing disulfide bonds.
2. Linkers between consecutive N- and C- termini. (The structure shows that the N- and C- termini of gp120 are relatively close together. A genetically constructed flexible linker of amino acids between the C- terminus of one monomer and the N- terminus of an adjacent monomer would also serve to covalently stabilize the oligomer.)
3. A gp140 construct (the extracellular portion of gp120 + gp41) with a mutation at the gp120/gp41

consensus cut site.

4. Trimers of GCN4 have been shown to enhance oligomerization. These oligomerization stabilizers could be added t the C-terminal tail of gp120.

Loop deletions:
Replacement of V1/2 loop with tripeptide Gly-Ala-Gly to expose of the CD4 binding site. Replacement of the V3 loop as well.

Stabilization of kinetically hidden epitopes of gp120. This invention uses gp120 which has been stabilized to elicit an immune response. gp120 may undergo conformational changes. However, only very few expose a conserved, neutralization epitope. This invention aims at using the information from the structure of gp120 to stabilize the hidden neutralization epitope of gp120. Specifically, the epitope may be stabilized by mutating the gp120 or alternatively, some epitope may be stabilized by ligand/drug interaction.

Specific examples are illustrated below:

Example 1:

The pocket of gp120 (Figure 51) only forms upon CD4 binding. If the residues along the pocket are mutated and was filled up, making it "stuck" in the CD4 conformation even without the binding CD4. Such mutation may include changing the Ser375 to Trp375, Val255 to Phe255 and Thr257 to Trp257.

The residues which lines the pocket include:
Trp 112 Leu 116 Pro 118 Phe 210 Val 255 Thr 257 Ser 375 Asn 377 Phe 382 Ile 424 Met 426 Trp 427 Asn 428 Ala 433 Gly 473 Met 475

Example 2:

Making disulfide bridges which tie protein domains. The

Topology for gp120 (Δ82, ΔV1/2, ΔV3, ΔC5) is shown in Figure 52. One can see the two domains, the N/C termini including α1, and a barrel around α2. A disulfide formed between ß2 and ß21 will tie the protein domains. As another example, disulfide bridge may be formed between ß5 and ß6 connection and top of the barrel (e.g. ß10).

Example 3

Cavities internal to the gp120 may be determined after knowing the three-dimensional structure of gp120. Analysis of all atoms are within 4 Angstroms of the surface defining each cavity allows mutations to be designed to determine if any large substitutions are allowed. Below shows some example of the analysis:

Val225 to Trp - not as good as 375 (below) -modeling shows some clashes with Met 475, although 475 should be able to move.

Ser375 to Trp - good fit (Note:the ser 375 mutation is incompatible with the Val225 mutation so only one can be made at a time).

Following are the antibody binding results:

<u>Table: Binding of the gp120 Variants to CD4BS Antibodies</u>

		CD4BS antibodies			
Mutants	F105	15e	IgGb12	21h	F91
255V/W	0.0	0.06	0.51	0.80	0.76
375S/W	0.0	0.36	0.05	0.72	0.0

Wild-type phenotype is 1.00 and decreases in recognition of below 1.

<u>Control for CD4 and 17b Binding</u>

Mutants	CD4	17b
255V/W	0.7	0.8
375S/W	0.9	1.0

The above result shows clearly that the mutations of Val255 to Trp, and Ser375 to Trp cause decrease of

binding to CD4BS antibodies.

The cavity filling mutant 375S/W clearly exhibits reduction in binding of CD4-BS antibody binding. While the data look good, two of the CD4-BS antibodies (15e and 21 h) still bind with reasonable affinity.

The basic idea behind the cavity filling mutants is to stabilize the CD4-bound conformation of gp120 at the expense of the CD4-free conformation. Additional substitutions may then be made in combination with the 375S/W. For example, taking the known mutations which exhibit similar phenotypes to 375S/W (See Thali et al (1995), J.Virol. 67, 3978-3988).

88N/P:Since this substitution is very far from the CD4 interacting surface, the only way to explain the results is they affect the C1/C5 terminal regions which in some manner affect the relative stability of the gp120 conformations.

102E/L: This glutamic acid is on the surface of gp120 and appears to stabilize the alpha1/alpha5 helix interaction. However, the stabilization is weak. The only way to explain the observed phenotype is that in the CD4-minus conformation, the glutamic acid is somehow involved in a stabilizing interaction, perhaps to the nearby Arg that in this conformation is just out of reach.

113D/R: The aspartic acid stabilizes the bridging sheet residues Gln428 and Lys429, which are important for maintaining the CD4-bound conformation of gp120.

117K/W: The lysine helps stabilize the bridging sheet conformation, but this substitutions may also affects CCR5 binding so it may not be so good a choice.

257T/A: Since this Thr is basically buried in the CD4-bound conformation, and indeed provides stabilizing hydrogen bonds, the only way to explain the phenotype of the T/A substitution is that Thr257 must be a critical element in maintaining the CD4-minus conformation. The residue is quite close 375W, so there may be some complications. If one places 375W in its preferred rotamer conformation, it clashes with Thr257-the mutation is accommodated by a slight change in rotamer conformation or by movement of the 375 backbone). So the T/A may actually help to accommodate the 375W change.

266A/E: The alanine is buried in the interface between the inner and outer domain. The substitution (on the face away from CD4 binding) most certainly effects thins conformationally, but since it is disruptive it is difficult to interpret.

386N/Q: This substitution is on the outer face of the outer domain and may not affect conformation. However, it does effect 21h the epitope of which is closer tot he inner domain so perhaps the loss of carbohydrate has long-range conformation effects.

395W/S: This substitution is also on the outer face of the outer domain. But it affects all the CD4-BS antibodies while retaining good CD4 binding.

421K/L: This is on bridging sheet. In the CD4-bound conformation, the Leu may pack nicely against Ileu423. Although this substitution may reduce CCR5 binding, the fact that it is far from where CD4 binds suggest that its effects may be conformational. (The effect 421K/D on CCR5 binding may be primarily electrostatic.)

470P/G and 475M/S: Both of these are close to the CD4-

binding region, although both are buried and do not interact directly with CD4. Both retain good CD4 binding so the effect may be conformational.

485K/V: This is at the inner/outer domain interface. There may be steric clashes of the valine (the base of the Lys is buried) which may be disruptive.

This invention further provides vaccine design based upon confromational stabilization using the three-dimensional structure. See e.g. Malakauskas and Mayo Nature Structure Vol.5, p.470-475, entitled "Design, Structure and Stability of a hyperthermophilic protein variant," the content of which is incorporated into this application by reference.

The invention will be better understood by reference to the Experimental Details which follow, but those skilled in the art will readily appreciate that the specific experiments detailed are only illustrative, and are not meant to limit the invention as described herein, which is defined by the claims which follow thereafter.

FIRST SERIES OF EXPERIMENTS

Probability analysis of variational crystallization and its application to gp120, the exterior envelope glycoprotein of type 1 human immunodeficiency virus (HIV-1)

Summary

The extensive glycosylation and conformational mobility of gp120, the envelope glycoprotein of type 1 human immunodeficiency virus (HIV-1), pose formidable barriers for crystallization. To surmount these difficulties, we used probability analysis to determine the most effective crystallization approach and derive equations which show that a strategy, which we term variational crystallization, substantially enhances the overall probability of crystallization for gp120. Variational crystallization focuses on protein modification as opposed to crystallization screening. Multiple variants of gp120 were analyzed with an iterative cycle involving a limited set of crystallization conditions and biochemical feedback on protease sensitivity, glycosylation status, and monoclonal antibody binding. Sources of likely conformational heterogeneity such as N-linked carbohydrates, flexible or mobile N- and C-termini, and variable internal loops were reduced or eliminated, and ligands such as CD4 and antigen-binding fragments (Fabs) of monoclonal antibodies were used to restrict conformational mobility as well as to alter the crystallization surface. Through successive cycles of manipulation involving 18 different variants, we succeeded in growing six different types of gp120 crystals. One of these, a ternary complex composed of gp120, its receptor CD4, and the Fab of the human neutralizing monoclonal antibody 17b, diffracts to a minimum Bragg spacing of at least 2.2 Å and is suitable

for structural analysis.

Introduction

In conventional crystallizations of biological macromolecules, the protein or other macromolecular subject is treated as a fixed entity to be tested in a multitude of crystallization conditions. Despite advances such as sophisticated screening procedures(1,2) and crystallization robots(3,4), this approach often fails for components from complex biological systems. One of these, the subject of this study, is the HIV-1 exterior envelope glycoprotein, gp120. In such cases, success may follow if the protein itself is varied. There are, however, many options in this vein and it is not clear how they might be prioritized. By way of background for this study, we first consider various options for the crystallization of conformationally complex macromolecules and then describe the characteristics of gp120.

Crystallization by variation and modification. For the more difficult crystallization challenges, which can be defined as those for which conventional screening fails, one typically tries to vary or modify the protein while maintaining biologically important properties. Meaningful results obtain since the integrity of internal structure and functional properties can often tolerate variation at the molecular surface where lattice contacts are made. The probability for success in crystallization is enhanced because flexible or heterogeneous surface features may be removed or because of the fortuitous introduction of lattice interactions. A prescient example that pre-dates the powerful methods of modern molecular biology was John Kendrew's screening of myoglobins from many different organisms until he found one, from sperm whale, that crystallized well(5).

Indeed, human myoglobin requires a Lys to Arg substitution in order to produce crystals suitable for structural analysis(6). Conversely, crambin forms exceptionally well-ordered crystals despite being a mixture of two isoforms with sequence variation at internal residues(7).

There are many notable examples of variation or modification in the crystallization of macromolecules. Systematic variation in the species of origin, as pioneered with myoglobin(5), was also instrumental in the crystallization of the transcription initiating TATA-binding protein(8). Proteolysis is often used to define crystallizable fragments, following the early examples from enzymatic digestions of antibodies that produced crystallizable fragments (reviewed in (9)) and the bromelain release of hemagglutinin from the influenza virus membrane(10). Variation of recombinant constructs, often inspired by proteolytic definition, is now commonplace with the widespread use of molecular biology tools. Systematic variation in the length of DNA oligomers has proved essential in the structural studies of protein - nucleic acid complexes. The work of Jordan and Pabo on λ repressor(11) sets the example for transcription factors, and the principle extends to other complexes as for the nucleosome(12). The use of protein ligands to stabilize another protein of interest for crystallization has also been effective as in the study of actin through its complex with DNase I(13) and more generally through complexes with antigen-binding Fab fragments of antibodies (reviewed in (14)). The principle that the detergent solubilized lipid interface of membrane proteins is generally unavailable for lattice contacts has led to the concept that crystallizability will be enhanced if the non-variable surface area is increased, and this was demonstrated in practice in the crystallization of a bacterial

[redacted]

cytochrome oxidase in complex with an antibody Fv fragment(15). Similarly, the anticipated conformational and compositional heterogeneity in carbohydrate moieties of glycoconjugates is expected to interfere with crystallization, and deglycosylation has proved essential for heavily glycosylated proteins such as human chorionic gonadotropin(16).

Characteristics of HIV gp120. HIV-1 induces acquired immunodeficiency syndrome (AIDS) in humans(17,18). The gp120 glycoprotein helps to mediate virus entry into cells through sequential recognition of two cellular receptors, the surface glycoprotein CD4(19,20) and a chemokine receptor (primarily CXCR4 or CCR5, depending on viral strain)(21-26). These high affinity interactions are attractive targets for mimetic drug design. Although the structure of the gp120-binding domain of CD4 and the identity of residues critical to its interaction with gp120 have been known for several years(27,28), this has not been sufficient for design of potent antagonists(29-31). As the major virus-specific antigen accessible to neutralizing antibodies, knowledge of the gp120 structure could also impact considerably on vaccine design. Despite this interest and considerable effort for several years with pure soluble protein, available in quantities as a byproduct in part from vaccine trials, gp120 has resisted crystallographic analysis.

The mature gp120 glycoproteins of different HIV-1 strains typically have 470-490 amino acid residues(32). Extensive N-linked glycosylation at 20-25 sites accounts for roughly half of the gp120 mass(32,33). Sequences from many different viral isolates show that gp120 has five variable regions (V1-V5) interspersed between relatively conserved regions (C1-C5)(32,34) and nine conserved disulfide bridges(33). Except for limited N-

and C-terminal cleavage, proteolytic digestion does not reveal a sub-domain structure. Indeed, even after extensive proteolytic cleavage, the unreduced protein runs near its native molecular weight on SDS-PAGE (PDK, unpublished data).

The gp120 glycoprotein likely exhibits conformational flexibility. Some of the variable regions, the V2 and V3 loops in particular, are known to be exposed on the surface of the native protein and probably assume multiple conformations. The potential of gp120 to undergo conformational change is also evidenced by shedding, the CD4-induced dissociation of gp120 from the surface of the virus, by ligand-induced variations in monoclonal antibody binding(35,36), and by complex CD4-gp120 binding kinetics(37). These changes may be related to the functional role of gp120 in virus entry.

The extensive glycosylation and conformational heterogeneity of gp120 suggested that merely screening the protein through ever more exotic crystallization conditions would not produce well-diffracting crystals. We have analyzed the effectiveness of optimizing different crystallization factors given the specific characteristics of gp120. This led us to a strategy employing radical modification of the protein surface, primarily to reduce heterogeneity but also to create new potential lattice contacts. We derive equations which show that this strategy, which we term variational crystallization, substantially enhances the overall probability of crystallization for gp120. An iterative process, involving both biochemical and molecular biological techniques, was used to detect and remove chemical and conformational heterogeneity. In addition, protein ligands, namely CD4 and the Fab fragments of several monoclonal antibodies, were used to restrict conformational mobility. Progressive trials of 18

different gp120 crystallization variants yielded six different crystals, at least one of which is suitable for structural analysis. This paradigm of crystallization, with a focus on protein modification rather than on crystallization screening, may aid in the structural analysis of other conformationally complex proteins.

Theoretical Analysis

Much of the crystallization literature is anecdotal, reflective perhaps of the diverse nature of proteins. Systematic quantitative studies have necessarily focused on robust, well characterized systems(38). If a particular protein fails to crystallize, one is faced with a bewildering array of options based on the experience with other often quite different proteins. In the absence of a comprehensive crystallization theory it is difficult to know how to proceed. Here, we devise an approximate theoretical underpinning for such decisions based on the ratio comparing crystallization probabilities before (P_i) and after (P_f) a modifying procedure. We define the enhancement in crystallization probability as $\mathcal{E} = {}^{Pf}/_{Pi} - 1$ whereby $\mathcal{E} = 0$ for no change and can reach a maximum, $\mathcal{E}_{max} = 1/P_i - 1$, that depends on the inverse of the initial probability.

In evaluating different crystallization strategies, one important consideration is effectiveness. Many factors affect crystallization, and a suitable crystallization approach depends on identifying and dealing with those that are most limiting. For example, if a protein were only 30% pure, the crystallization probability associated with such protein purity would be low and a purification strategy would be key; if a protein were 98% pure, further purification would most likely have

little impact on the overall probability of crystallization. Factors that might be expected to affect the crystallization of gp120 are listed in Table 1, along with estimates of the effect of optimizing each factor given the specific characteristics of gp120.

Although identification of limiting crystallization factors can establish rough guidelines as to the appropriateness of a particular crystallization strategy, a better way to evaluate effectiveness (or perhaps to judge the progress of a specific crystallization effort) is by quantitative assessment of the enhancement in crystallization probability. For example, if 80% of all crystallizable proteins crystallize from a core set of 50 conditions(2), a strategy that involves screening ever larger arrays of crystallization conditions could at most enhance the probability of crystallization by only 25% over that for the first 50 conditions; further screening would yield increasingly diminishing returns. With this screening example, the quantitative enhancement of probability is straightforward to calculate, but it is not immediately apparent for the strategy of variational crystallization, which focuses on protein modification. We can consider two kinds of such modifications -- those designed to reduce heterogeneity and those related to expanding the number of crystallization candidates.

Enhancement of surface homogeneity. Crystalline order is explicitly dependent on lattice homogeneity. Reducing heterogeneity can be thought of as increasing the proportion of surface area available for formation of lattice contacts, increasing the probability of crystallization. The probability that a single lattice contact between two molecules may form is in part related to the fraction of surface area that is homogeneous on one molecule multiplied by the fraction

homogeneous on the other, i.e.,

$$P(\text{homogeneous contact}) \propto H(\text{molecule } 1) \times H(\text{molecule } 2) \quad (1)$$

where H is defined as the homogeneous fraction of the surface. Consider the case where the molecule in question is the smallest repeating unit in a crystal, that is, the asymmetric unit. In such a case molecule 1 and molecule 2 are equal, and the above equation reduces to (% homogeneous surface)^2. Now consider the same scenario with two lattice contacts; the probability that both are homogeneous is related to $[(H-\partial_{\bar{1}})^2 \times (H-\partial_2)^2]$ where "H" is the homogeneous fraction of the surface which may form lattice contacts and "$\partial_{\bar{n}}$" is a function of the relative size and total number of lattice contacts other than contact *n* and the degree and distribution of surface homogeneity -- related to the occlusion of available surface area upon formation of each lattice contact as well as the spatial distribution of homogeneous surface over the molecular surface. Generalizing to case of "C" lattice contacts, the probability associated with homogeneous lattice formation is related to:

$$P(\text{latice}) \propto [(H-\partial\bar{1})^2 \times (H-\partial_2)^2 \times \ldots \times (H-\partial c)^2] = \prod_{n=1}^{C} (H-{}_{\partial}\bar{n})^2] \quad (2)$$

In the restricted case of one molecule per asymmetric unit, the observed average value of "C" (C_{ave}) is ~4.5(39), with a minimum theoretical value for the most common space groups of 2 or 3(39). Since C may be relatively small, lattice contacts may make up only a small proportion of a macromolecule surface, with considerable surface heterogeneity tolerated. Thus, for example, many proteins that pack into well-ordered

crystal lattices have disordered regions, with N- and C-termini as well as internal loops being unresolved.

Given a reduction in surface heterogeneity, what is the change in crystallization probability? Surface area is correlated with molecular mass (M) by the power law: surface area = 6.3 x $M^{0.73}$, which on average predicts surface area to within 4% for monomeric proteins (40). The fraction of homogeneous surface can thus be approximated as a ratio of molecular masses of the total and of the homogeneous portion of the protein:

$$H \approx [M(\text{homogeneous}) \ / \ M(\text{total})]^{0.73} \qquad (3)$$

From Eqs. 2 and 3, it is now possible to estimate the enhancement in probability for crystallization upon reduction of heterogeneity. With the simplifying approximation $\partial\bar{n}\approx 0$, the probability ratio of before($\mathbf{P}_i$) and after($\mathbf{P}_f$) becomes

$$^{Pf}/_{Pi} \approx [(M(\text{homogeneous})f \ / \ M(\text{total})f]^{1.46 \times C} \ / \ [(M(\text{homogeneous})i \ / \ M(\text{total})i]^{1.46 \times C} \qquad (4)$$

Equation 4 is still not very useful, however, since M(homogeneous) is unknown and molecule-specific. In reducing heterogeneity, however, it seems reasonable to assume that the removed portion, if it were a highly branched carbohydrate or a proteolytically exposed region, is completely heterogeneous. In such cases, [M(homogeneous)f ≈ M(homogeneous)i] whether or not all heterogeneity has been removed. Assuming that $C \approx C_{ave}$, the enhancement ($\mathcal{E}$) in probability on removal of a heterogeneous portion becomes

$$\mathcal{E}_r = {}^{Pf}/_{Pi} - 1 \approx [\ M(\text{total})i \ / \ M(\text{total})f]^{1.46xC_{ave}} - 1 \qquad (5)$$

This last equation allows the change in crystallization probability upon heterogeneity removal to be quantified. For example, consider a situation where a recombinant DNA approach is used to produce a protein with an affinity tag of 10 amino acid residues. Is it important to remove these presumably flexible residues? From Eq. 5, the answer depends on the protein size. For a 100-residue protein, removal of the tag would greatly enhance the crystallization probability by: $\mathcal{E}_r = {}^{Pf}/_{Pi} -1 \approx [110/(110-10)]^{1.46 \times 4.5} -1 = 0.87$, or almost 90%, whereas for a 500-residue protein the enhancement would be minimal, $\mathcal{E}_r = 0.14$.

Another variant of Equation 4 can be used to estimate the impact of adding a ligand of fixed structure to a molecule that contains heterogeneous portions. This expands the surface available for lattice contacts and effectively dilutes the heterogeneous component. It may be an approach of choice when the heterogeneity is essentially unremovable, such as at the lipid interface of detergent solubilized membrane proteins. One faces the difficulty of estimating the extent of heterogeneity to use Eq. 4, but this might be done by summing the residual variable components in gp120 or by topographical estimates for a membrane protein. (For example, for a sphere embedded symmetrically in a membrane of thickness h, $1-H = \text{area(heterogeneous)}/\text{area(total)} = h/[6Mv/(\pi N_o)]^{1/3}$, where M is molecular mass, v is partial specific volume and N_o is Avogadro's number. Thereby, $1-H = 0.62$ for $h = 30Å$ and $M = 50$ kDa.). Then the enhancement in probability on addition of a fixed component becomes

$$\mathcal{E}_a = \{[M(\text{total})i / M(\text{total})f] \times [M(\text{total})f - M(\text{hetero})i] / [M(\text{total})i - M(\text{hetero})i]\}^{1.46 \times c_{ave}} -1 \qquad (6)$$

In the instance of a 50 kDa protein, half of which is heterogeneous, to which a 25 kDa Fv fragment is complexed, $\mathcal{E}_a=\{[50/75]\times[75-25]/[50-25]\}^{1.46 \times 4.5} -1 = 5.6$. Thus if the overall crystallization probability of the protein was initially only 1 chance in 10, assuming all other crystallization probability components remained unchanged, the crystallization probability of the Fv fragment complex would be roughly 1 chance in 2, a substantial enhancement.

The accuracy of the quantification is only as good as the approximations, and several of the approximations used here call for further scrutiny. The approximation of molecular mass for surface area was used for the initial protein prior to heterogeneity removal. This is probably an underestimate since the completely heterogeneous portions of the protein would not be expected to fold as compactly as the homogeneous portions. In addition, the approximation that $\partial\tilde{n}\approx 0$ tends to underestimate the deleterious influence of heterogeneity on crystallization. Both of these assumptions show an underestimation, but the equations still should predict the correct general trend. For some assumptions, however, the effect is more subtle. For example the equations were generated assuming one molecule per asymmetric unit. If one considered a tight complex of molecules, the same equations would hold as long as the complex did not have internal symmetry (complexes with internal symmetry show a different average contact number). Finally the category of heterogeneity is quite broad, and there are some situations, such as with segmental flexibility where these equations may be invalid. For example in the case of two rigid domains connected by a flexible linker, one would have to consider the possibility that one domain could be fixed relative to the other with a single appropriate contact.

Increase of molecular variants. Another aspect of variational crystallization, the use of multiple variants of the same protein, also increases the probability of crystal formation. In this case, the overall probability of crystallization is exponentially related to the number of variants. Assuming independence of variants (a reasonable assumption with different protein ligands; not as valid with minor changes) with n variants and a probability of crystallization for each variant of P_i, the overall probability P_T is:

$$P_T = 1-[(1-P_1) \times (1-P_2) \times \ldots \times (1-P_n)] = 1- \prod_{i=1}^{n} (1-P_i) \qquad (7)$$

For example, if each variant of a relatively heterogeneous protein had only a 25% chance of crystallizing, the overall probability would be $1-(1-0.25)^n$; with 15 variants, the probability would increase to almost 99%.

The enhancement in overall probability for successful crystallization from a set of n variants can then be calculated relative to the probability for a single variant. If we assume that the probability for crystallization of this individual variant, i, is typified by the average for all variants, $P_i \approx P_{ave}$, the enhancement factor is

$$\mathcal{E} = {}^{P_T}/_{P_i} - 1 \approx ({}^{1}/_{P_{ave}}) - [(1-P_{ave})^n/_{P_{ave}}] - 1 \qquad (8)$$

If one tries many variants such that $(1-P_{ave})^n \ll 1$, then the enhancement is inversely related to the average probability of crystallizing a single variant:

$$\mathcal{E} \approx ({}^{1}/P_{ave}) - 1 \qquad (9)$$

Thus, the more difficult a protein is to crystallize, the more it benefits from a strategy employing multiple variants.

Experimental Procedures

Constructs of gp120. The various recombinant gp120 glycoproteins used for crystallization trials were produced in stable *Drosophila* Schneider 2 lines under the control of an inducible promoter as previously described(41) (Table 2). Genetic constructs containing various deletions and substitutions were made during the course of dissecting the gp120 domain structure. The procedures for making these constructs and the biological properties of the corresponding protein products are described elsewhere (see references in Table 2).

Protein production and purification. The N-terminal two domains of CD4 (D1D2), residues 1-183, were produced in Chinese hamster ovary (CHO) cells and purified as described previously(27). Human monoclonal antibodies 17b, A32, C11 and F105 (derived from HIV-infected individuals)(42,43) and mouse monoclonal antibodies L71 and 178.1(44,45) were purified by Protein-A affinity chromatography. Secreted gp120 from *Drosophila* cells was purified by affinity chromatography with the F105 antibody covalently coupled to Sepharose. Following extensive washing with phosphate-buffered saline containing 0.5 M NaCl, gp120 protein was eluted with 0.1 M glycine, pH 2.8, followed by immediate neutralization with Tris buffer.

Protease Digestion. Fab fragments were produced by papain digestion of monoclonal antibodies. Briefly, the antibody was reduced in 100 mM DTT, 100 mM NaCl, 50 mM

Tris pH 8.0 for 1 hr at 37°C, and dialyzed (4°C), first in phosphate-buffered saline (PBS) to reduce the DTT concentration to ~1 mM, then in alkylating solution (PBS titrated to pH 7.5 with 2 mM iodoacetamide, 48 hr), and subsequently in PBS without iodoacetamide. The reduced and alkylated antibody was concentrated to at least 2 mg/ml and digested with papain using a commercial protocol (Pierce). An additional gel filtration chromatographic step on a Superdex S-200 column (Pharmacia, FPLC) was added to ensure oligomeric homogeneity.

The gp120 proteins were subjected to digestion with papain, elastase, and subtilisin (Boehringer Mannheim) to assay for proteolytic susceptibility. In these assays, the gp120 concentration was kept constant and the protease diluted serially (3.3x) from a ratio of 1:10 to 1:1000. The digestion mix was incubated for 1 hr at 37°C and quenched by addition of 1% SDS (1:10 ratio) with immediate heating in boiling water for 2 minutes. Digestion products were analyzed with SDS-polyacrylamide gel electrophoresis (PAGE) with and without DTT reduction.

Carboxypeptidase Y digestion was used to analyze the C-terminus of gp120. A 1:10 ratio of carboxylpeptidase Y (Boehringer Mannheim) to gp120 was incubated for 1 hr at 37°C, pH 7.0. Even though digestion could not be easily seen by SDS-PAGE, the C-terminus of gp120, HXBc2 strain, contains a number of positively charged amino acids, and the extent of the reaction could be monitored by native-PAGE.

Deglycosylation. *Drosophila*-produced gp120 proteins were deglycosylated enzymatically. Briefly, 0.5 mg/ml of gp120 was incubated with various deglycosylating enzymes (singly or in combination) in 0.5 M NaCl, 100 mM

Na acetate, pH 5.7, for 10 hr at 37°C. Endoglycosidase D was used at a concentration of 0.1 U/ml, Endoglycosidase F at 0.25 U/ml, Endoglycosidase H at 0.25 U/ml, and Glycopeptidase F at 0.1 U/ml (all from Boehringer Mannheim). For crystallization variants involving the CD4-gp120 complex, the addition of D1D2 (which lacks carbohydrate) to the deglycosylation cocktail was found to enhance gp120 solubility. The deglycosylation reactions were monitored by following the reduction in molecular weight on SDS-polyacrylamide gel electrophoresis (SDS-PAGE). Deglycosylation was nearly complete within 30 min and plateaued after 3 hr. The extent of deglycosylation was judged by matrix-assisted laser desorption (MALDI) mass spectroscopy, carbohydrate analysis, affinity for concanavalin-A, and mobility and band width on SDS-PAGE. Protein aggregation was assayed by native-PAGE, dynamic light scattering, and gel filtration chromatography.

Monoclonal antibody binding assay. The various gp120 glycoproteins were assessed for recognition by a variety of monoclonal antibodies directed against both linear and discontinuous gp120 epitopes by either immunoprecipitation(46) or by ELISA(47). The ELISA was performed with both fully glycosylated and deglycosylated ΔV1/2ΔV3 glycoproteins immobilized on ELISA plates using a capture antibody specific for the gp120 carboxyl-terminus, 6205 (International Enzymes)(47).

Binary and ternary complex purification. To ensure proper stoichiometry and oligomeric homogeneity, all complexes were purified by gel filtration chromatography on a Superdex S-200 column (Pharmacia, FPLC). This column exhibited good resolution with routine separation of samples that differed by only 30% in molecular weight. Individual components were first purified

separately to ascertain their monomeric status. Components were then combined to form complexes, which were repurified on the same column. A buffer of 0.35 M NaCl, 5 mM Tris/Cl pH 7.0, 0.02% NaN_3 was used throughout. Peak fractions were concentrated over centricon-30 (Amicon) to a final protein concentration of ~10 mg/ml and either aliquoted and stored at -80°C or used directly for crystallization.

Crystallization. The vapor-diffusion hanging-droplet technique was used for all crystallizations. Small volumes, 0.5 μl protein solution + 0.5 μl reservoir solution, were used for most crystallizations, screenings and final optimizations.

Screening. The Crystal Screen I (Hampton Research) was used, augmented by approximately 20 conditions which tested high protein concentrations (vapor diffusion concentration of the protein at various pHs) as well as mixtures of organic additives (2-5% MPD, PEG 400, or PEG 4000) combined with high ionic strength (2-4 M NaCl, $(NH_4)_2SO_4$ or Na/KPO_4) at pH 5.5-9.5. For each gp120 crystallization variant, a subset of 12 different conditions was analyzed in depth to establish the approximate precipitation point of the protein for a variety of different precipitants. The factorial solutions were then individually adjusted to target the observed precipitation point and a full screen of ~70 conditions was set up at 20°C. After at least one week of constant daily observation, screening solutions were recalibrated to account for the observed 20°C precipitation point and another full screen at 4° C was set up. If no crystals were observed, the Crystal Screen II (Hampton Research) was set up at 20° C.

Optimization. In addition to the standard single variable optimization of crystallization conditions, a

factorial-like procedure was used to determine if small amounts of different additives increased crystal quality. Type E crystals were grown from the following conditions: Protein (Δ82ΔV1/2*ΔV3ΔC5 gp120, two-domain CD4 (D1D2), Fab 17b purified as a ternary complex on the Superdex S-200); Droplet (0.5μl protein solution consisting of ~10 mg/ml protein in gel filtration buffer + 0.4 μl droplet mix containing 0.1 M NaCitrate, 0.02 M NaHepes, 10% isopropanol, 10.5% PEG 5000 monomethylether (Fluka), 0.0075% SeaPrep Agarose (FMC BioProducts), pH 6.4; Reservoir: (0.35 M NaCl, 0.1 M NaCitrate, 0.02 M Hepes, 10% isopropanol, 10.5% PEG 5000 monomethylether, pH 6.4). The droplet mix was kept at 37°C to ensure the agarose solubility, and the crystallization setup at room temperature. Clumps of crystals appeared within two weeks of incubation at 20°C and grew for several months to maximal size.

X-ray diffraction characterization. All data were collected at beamline X4A of the National Synchrotron Light Source, Brookhaven National Laboratory. The type E crystals were crosslinked with the vapor diffusion technique of Lusty(48) by placing a crystallization bridge (Hampton Research) with a 25 μl sitting droplet of 1% glutaraldehyde (Sigma) in the reservoir of a standard hanging droplet vapor diffusion crystallization setup for 1 hr at room temperature. The crosslinked crystal was washed with stabilizer (reservoir solution with only 50 mM NaCl) containing 10% ethylene glycol. After approximately 24 hr, the external liquid surrounding the crystal was replaced with paratone-N (Exxon), the crystal mounted in an ethylene loop (Hampton Research)(49), and flash-cooled in the nitrogen stream of a cryostat (details are provided in (50)). Oscillation data were processed with DENZO(51) and scaled with SCALEPACK(51).

Results and Discussion

To address the many problems associated with the crystallization of HIV-1 gp120, we exploited the mutability of the macromolecular surface using tactics that involved protein modification and conformational restriction (Table 3). Several of these tactics contain novel features and are detailed here.

Variant constructs of the gp120 protein. Variants of gp120 were developed through an iterative cycle which strove to eliminate heterogeneity. The cycle involved recombinant production of gp120 variants, deglycosylation, and then assessment of heterogeneity and flexibility by examinations of glycosylation status, monoclonal antibody binding, and protease sensitivity, leading to the design of new constructs. For example, protease digestion monitored by PAGE indicated susceptibility at the C-terminus, and a form with 15-20 residues removed by carboxypeptidase Y retained CD4 binding activity. A homogeneous product was difficult to make by this method, and primer-based PCR mutagenesis and recombinant expression were used to generate a homogeneous gp120 derivative with a 19-residue C-terminal deletion. At the N-terminus, sequencing of the initial constructs showed the expected signal cleavage at +31, with four additional amino acids, Gly-Ala-Arg-Ser, added from the signal peptide (a consequence of different processing of the cloning vector signal peptide with gp120). Protease digestion gave a product at +40, indicating flexibility in the N-terminus. Progressive genetic truncation and biochemical analysis identified +83 as a variant that was recognized by conformation-dependent gp120 ligands, whereas +94 exhibited some conformational disruption(46). Thus much of the apparently flexible region at the N-terminus of gp120 could be removed

without disrupting the global conformation of the protein.

To further reduce flexibility, variable loops, V1, V2, and V3, were deleted and replaced with shorter segments, as reported earlier (52,53). Little effect was found on CD4 binding activity(47,53). Three constructs were made which contained deletions of the V1, V2, and V3 loops (Table 2). In the ΔV1/2ΔV3 construct, the entire base and stem of the variable loops V1, V2 and V3 were excised. In the ΔV1/2*ΔV3 protein, the conserved stem of the V1/V2 stem-loop structure was retained, restoring the CD4-induced antibody epitopes in the presence of soluble CD4. In the ΔV1/2*ΔV3* protein, the base of the V3 loop was retained as well, fully restoring CD4-induced antibody epitopes, even in the absence of soluble CD4.

Deglycosylated forms of gp120. The asparagine-linked carbohydrate on the gp120 glycoprotein produced in *Drosophila* cells was analyzed. Dionex chromatography showed that the carbohydrate on this protein consisted of (N-acetyl-glucosamine)$_2$ (fucose)$_F$ (mannose)$_M$, with F = 0 or 1 and M = 3 to 9 (JSC, unpublished data). Deglycosylation with enzymes such as Glycopeptidase F (or Endoglycosidase F at pH 5.0), which cleave the glycosidic linkage and convert the N-linked asparagine into an aspartic acid, resulted in gp120 aggregation, although it remained soluble. Cleavage of the 1-4 β-bonds in the chitobiose core with Endoglycosidases D or H, leaving only a single N-acetylglucosamine residue and, potentially, a 1-6 fucose attached to any of the glycosylated asparagine residues, appeared to leave the protein intact as judged by a panel of conformationally sensitive monoclonal antibodies(47). Digestion of full-length constructs with Endoglycosidase H, which has specificity for oligosaccharides with 5-9 mannose

residues, removed roughly 60% of the carbohydrate, and addition of Endoglycosidase D, which cleaves oligosaccharides with 3 or 4 mannose residues, removed up to 90% of the carbohydrate. For the variable loop-deleted constructs, all mannose residues were removed with the Endoglycosidase D/H combination as judged by carbohydrate analysis and by the inability of concanavalin A to bind to the deglycosylated protein. Mass spectroscopy of the deglycosylated Δ82ΔV1/2*ΔV3ΔC5 gp120 showed a molecular mass of 39,000 ± 50 Da, consistent with a mass of 35.4 kDa for the protein (based on the DNA sequence) and 3.6 kDa for the remaining carbohydrate. Carbohydrate analysis showed only fucose and N-acetyl-glucosamine sugars to be present, in a ratio of 1:3.05 ± 0.02, respectively. These results suggest that, of the 18 potential asparagine glycosylation sites in the Δ82ΔV1/2*ΔV3ΔC5 gp120, five are unused, nine are modified with N-acetyl-glucosamine and four with N-acetyl-glucosamine (1-6) fucose.

Complexes with gp120 ligands. Protein ligands, CD4 and the Fab fragments of monoclonal antibodies, were used in an attempt to reduce mobility in the overall surface of the protein and, hence, in the potential crystal lattice. This was complicated by the internal mobility of these ligands: CD4 has a flexible juncture between the second and third extracellular domains(54), and Fabs have a conformationally mobile "elbow bend" between their variable and constant domains(55). For CD4, we used a construct containing the N-terminal two domains (1-182), for which we had previous success in structure determination(27). Fabs of the monoclonal antibodies, were screened individually, even though combinations of Fabs were possible.

Initial trials with the Fab 178.1, which recognizes a

linear epitope in V3 of both free- and CD4-bound gp120(44), gave only crystalline precipitates at best. We also tested the Fab of the anti-CD4 antibody L71, which recognizes the CDR3-like loop in domain D1(45), but had difficulties preparing ternary complexes, probably due to a destabilization of the CD4 - gp120 interaction. Subsequently, we focused on gp120-directed antibodies with discontinuous epitopes, which were more likely to recognize conformationally rigid portions of gp120. Complexes of gp120 proteins with Fabs of C11, which recognizes an epitope spanning C1 and C5(42), and F105, whose epitope lies within C2, C3, C4, and C5 (overlapping the CD4 binding site)(43) gave only poor crystals (Table 4). We had greater success with 17b, which not only recognizes a discontinuous epitope but discriminates between different conformational states of gp120(36). The Fab of 17b did not bind the initial gp120 constructs, requiring the restoration of the stem of the V1/V2 loop (constructs ΔV1/2*ΔV3 or ΔV1/2*ΔV3*).

Crystallization. We screened 18 different combinations of gp120 variants and ligands (Table 4), using a limited factorial-based crystallization screen. Factorial screening was originally devised as a method for deducing the essential crystallization factors from combinations of different conditions(1). The empirical observation, however, that most crystallizable macromolecules are able to crystallize from a limited set of common conditions, has validated an entirely different process: crystallization screening with a small but diverse collection of fixed conditions(2). A high probability of success has been reported with as few as 6 different conditions at 4 different concentrations(56), and commercial kits are available with 50-100 conditions (Hampton Research).

In conjunction with the limited crystallization screen,

small volume droplets were used, typically 0.5 μl of protein per crystallization trial. With small volumes, 1-2 mg of protein was sufficient to evaluate each gp120 crystallization variant. Smaller volumes were also more efficient at nucleation than larger droplets, perhaps due to higher surface tension effects which may result in a greater range of precipitant concentrations for each droplet to sample. Indeed, droplets that were "spread-out" also showed enhanced nucleation. This explanation may also account for the well-known observation that crystals frequently nucleate from the edges of crystallization droplets.

The initial crystallization screens produced six different types of crystals (Fig. 1, Table 5). For crystal types A-D, extensive optimization was unable to produce single crystals large enough to be characterized. For crystal types E and F, single crystals of needle morphology could be grown. The growth of single crystals of type E, however, required the addition of agarose, which was identified during optimization by the additive screening process. Trials with a variety of agaroses found the SeaPrep, with a gelling point near room temperature, gave the best results. Despite considerable effort, further crystallization optimization failed to produce large single crystals, and the best typical crystals were rods with a cross-section of only 30 x 40 μm. A closely related crystallization variant, which retained 10 additional amino acids in the stem of the V3 loop, failed to crystallize (Table 4).

Characteristics of gp120 crystals. Single crystals of type E and F were analyzed for diffraction in capillary mounts. Only type E crystals showed diffraction. The needle axis of type E crystals proved to coincide with the *a* axis, and the rhombohedral cross-section

perpendicular to the needle axis proved to be bounded by faces of the form (0 1 1). These could be distinguished from type F crystals, where the cross-section was hexagonal. Gel electrophoresis of type E crystals demonstrated that they contained all the elements of the ternary complex: gp120, D1D2, and Fab 17b (Fig. 2).

We were unable to flash-cool the type E crystals with standard cryoprotectants. Satisfactory results were found with a procedure that (i) fortified the crystals with vapor-diffusion glutaraldehyde crosslinking(48), (ii) permeated the crystals with 10% ethylene glycol and (iii) used an immiscible oil, paratone-N, to replace the external solution around the crystals prior to flash-cooling(50) Cryopreserved crystals diffracted to Bragg spacings of better than 2 Å, although the diffraction was anisotropic, with higher mosaicity along the 88 Å *b*-axis.

Type E crystals were orthorhombic, space group $P222_1$ with unit cell parameters, a=71.25Å, b=88.11Å and c=196.44Å ($\alpha=\beta=\gamma=90^\circ$). Solvent content analysis yielded a solvent content of 58% for one ternary complex in the crystallization asymmetric unit (assuming a partial specific volumes of 0.73 for protein and 0.65 for carbohydrate and the observed total molecular mass of 108.3 kDa for the complex of which 3.6 kDa is carbohydrate). Diffraction data have been collected to a limit of 2.2Å spacings (Table 6).

Conclusions. Our success with gp120 demonstrates the power of variational crystallization. We have derived equations that quantify the effect of this strategy on the overall probability of crystallization and have calculated the corresponding probability enhancements for several of the biochemical and molecular biological manipulations employed in this study. As can be seen

(Table 3), the probability of crystallization can be strongly influenced by reducing molecular surface heterogeneity. The influence of using multiple variants is more difficult to quantify since it depends on the individual probability of crystallization for each variant. Nonetheless, our theoretical analysis shows that the effect of multiple variants is greatest for proteins least likely to crystallize.

While the variational approach with gp120 did involve extensive effort, this was primarily a consequence of the difficulty in producing the gp120 glycoprotein, which involved expression levels of only a few mg of gp120 per liter of eukaryotic cell culture. While future advances in molecular biology will no doubt make such projects less arduous, if proteins are expressed bacterially, present day recombinant techniques coupled to affinity or "tag" purfications make the generation of variants straightforward. A recent example, involving the generation of 11 different variants in the crystallization of an ionotropic glutamate receptor(57), required only a 6 month effort (E. Gouaux, personal communication).

The resistance of gp120 to crystallization may be related in part to its functional role in eluding the immune system; the mechanisms evolved to prevent the formation of specific immune system : gp120 contacts, might also thwart formation of the homogeneous gp120 : gp120 contacts needed for crystallization. Perhaps relevant to this, the protein modifications that most greatly reduced heterogeneity (and thus enhanced the crystallization probability), removal of carbohydrate and substitution of the variable loops (Table 3), have been shown in vivo to enhance the generation of neutralizing antibodies(58,59).

It is difficult to evaluate the predictions of the crystallization algorithms derived here in a statistically significant manner. The failure of proteins to crystallize is rarely reported in the literature, and our own results comprise too small a sample to be statistically meaningful. Nonetheless, we note that for gp120 the algorithms predict that crystals are most probable with deglycosylation, variable loop removal, and addition of an ordered protein ligand. Consistent with prediction, for the 6 crystallization variants that did have all of these modifications, three (or 50%) produced crystals, whereas for the 12 variants that did not have these modifications, no crystals (0%) were grown. In addition, theory predicts that well-ordered crystals are most probable when the overall probability of crystallization is highest; Table 4 shows that the crystallization variant that produced the only well-ordered crystals appeared to have the greatest probability of crystallization, producing three different crystals forms whereas the best of the other variants only produced one form each.

The crystallization literature is replete with examples of protein manipulation, from proteolytic digestion, to variation in solvating detergent, to screening of DNA oligonucleotides(38). What distinguishes our efforts is the derivation of a theoretical foundation, which allows the probabilistic assessment of the most effective crystallization approach. Because of the conformational complexity of gp120, we focused on surface modification -- to eliminate heterogeneity and to present new crystallization variants -- coupled to a limited screen of crystallization conditions. The types of crystallization problems embodied in gp120 (Table 3) are not so different from many of the typical problems facing present day crystallographers; both from a theoretical or from a practical perspective, the

strategy of probability analysis coupled to variational crystallization may be broadly applicable.

Subsequent to the submission of this manuscript, the structure determination of type E crystals was reported(63).

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Table 1. Factors affecting the crystallization of gp120.

Crystallization factor	Specific gp120 characteristics	Optimization †
Protein characteristics:		
A. Chemical homogeneity		
-- other proteins	very clean -- affinity purification	+
-- carbohydrate variation	relatively limited, source dependent	++
-- polypeptide variation	N- and C- terminal ragged	++
B. Conformational heterogeneity		
-- carbohydrate	N-linked, large and flexible	++++++++
-- surface loop flexibility	total of ~130 amino acids are flexible	+++++
-- N- or C- termini	~30 amino acids are flexible	++
-- other	function-related conformational mobility	+++
Screening characteristics:		
A. Protein		
-- solubility	requires ~300 mM NaCl for solubility	++
-- stability	stable for over 1 week in cell culture	+
-- availability	~5 mg quantities	++
B. Screening variations		
-- protein homologues	many different gp120 isolates	+++
-- ligands	many ligands (dozens of monoclonal antibodies available)	++++++

† Estimate of the effect on the crystallization probability of a strategy which optimizes the particular factor. The number of (+) symbols denotes the size of the effect: (+) refers to almost no change in probability after optimization, whereas (+++++) refers to a large change in probability. The scale used here is a qualitative estimate; for more quantitative results, see Table 3. For chemical heterogeneity, optimization refers to the effect on crystallization of making the protein more chemically homogeneous. For conformational heterogeneity, optimization refers to the effect of removing or circumventing the particular source of heterogeneity.

Table 2. The gp120 constructs used for crystallization.

construct name	gp120 strain †	amino acid for construct §	reference
Δ61-IIIB	IIIB	62-511	(59)
Δ30-FL	JRFL	31-511	(60)
ΔV1/2ΔV3	BH10/HXBc2	31-120 GAG 204-297 GAG 330-511	(53)
ΔV1/2ΔV3ΔC5	BH10/HXBc2	31-120 GAG 204-297 GAG 330-492	(61)
Δ82ΔV1/2*ΔV3ΔC5	HXBc2	83-127 GAG 195-297 GAG 330-492	(61)
Δ82ΔV1/2*ΔV3*ΔC5	HXBc2	83-127 GAG 195-302 GAG 325-492	(61)

† The ΔV1/2ΔV3 and ΔV1/2ΔV3ΔC5 constructs were chimeras of strains BH10 and HXBc2,
§ Sequence numbers refer to the translated gp160, with the mature gp120 beginning at +31. N-terminal sequencing showed that all constructs contained 4 additional amino acids, Gly-Ala-Arg-Ser, an artifact of the signal peptide cleavage. GAG here refers to the tripeptide, Gly-Ala-Gly, which was substituted for the removed amino acids.

Table 3. Crystallization problems, variational crystallization solutions, and enhancement of crystallization probability.

Problem	Solution	Probability Enhancement †
N-linked carbohydrate	Protein production in an inducible *Drosophila* cell line coupled with deglycosylation with Endoglycosidases D and H	1200%
Surface loop flexibility	Replacement of V1/V2 and V3 loops with tripeptide linkers of Gly-Ala-Gly.	370%
N- and C- terminal heterogeneity	Mutational deletion and proteolytic cleavage analysis coupled to the production of gp120 with truncated N- and C-termini	50% §
Conformational heterogeneity	Conformation restriction with protein ligands such as CD4 and Fabs from conformationally sensitive monoclonal antibodies	$({}^{1}/P_{ave}) - 1$ ¶

† The probability enhancement, ε, was calculated from the equation: $([\, MW(total)i \,/\, MW(total)f\,]^{1.46 \times C_{ave}} - 1)$ with $C_{ave}= 4.5$, the average observed contact number. For the drosophila produced HXBc2, the molecular weight for the glycosylated gp120 is approximately 90 kDa; the deglycosylated gp120, 60 kDa; and the deglycosylated ΔV1/2ΔV3 gp120, 47 kDa.

§ The N- terminus is resistant to proteolysis from +39 to +82, and thus probably adopts an ordered conformation. This number was calculated assuming only the C-terminal 19 and the N-terminal 8 amino acids were disordered.

¶ Dependent on the average probablity (P_{ave}) of crystallizing a single variant of gp120. If P_{ave}=10%, the use of many variants would lead to a probability enhancement of 900%.

Table 4. Summary of HIV-1 gp120 crystallization attempts

HIV-1 gp120 construct	glycosylation status §	cofactors †	comments#
Δ61-IIIB (IIIB strain)	glycosylated	—	bad precipitates
	~60% deglycosylated	—	bad precipitates
	~90% deglycosylated but some Asn to Asp	—	precipitates look better but still primarily bad
	~60% deglycosylated	D1D2 sCD4	ok precipitates
	~60% deglycosylated	Fab 178.1	ok precipitates
	~60% deglycosylated	D1D2 sCD4 and Fab 178.1	ok precipitates
	~90% deglycosylated	—	ok precipitates
Δ30-FL (JRFL strain)	~90% deglycosylated	—	ok precipitates
		D1D2 sCD4	ok to good precipitates
		Fab 178.1	good precipitates
		D1D2 sCD4 and Fab 178.1	good precipitates -- no crystals
ΔV1/2ΔV3 (BH10/HXBc2 strain)	fully deglycosylated	—	good precipitates -- no crystals
		D1D2 sCD4	very small, nice looking crystals in PEG 400 (Crystal Type A)
		D1D2 sCD4 and Fab C11	badly formed crystals from $(NH_4)_2SO_4$ (Crystal Type B)
ΔV1/2ΔV3ΔC5 (BH10/HXBc2 strain)	fully deglycosylated	D1D2 sCD4	spheroidal crystals in PEG 4000 (Crystal Type C)
		Fab F105	good precipitates -- no crystals
Δ82ΔV1/2*ΔV3ΔC5 (HXBc2 strain)	fully deglycosylated	D1D2 sCD4 and Fab 17b	three different types of crystals (Types D-F). Orthorhombic diffract to at least 2.2 Å
Δ82ΔV1/2*ΔV3*ΔC5 (HXBc2 strain)	fully deglycosylated	D1D2 sCD4 and Fab 17b	good precipitates -- no crystals

†D1D2 sCD4 refers to two-domain soluble CD4. Antibody epitopes are described in the text.

§The percent deglycosylation reported here refers to the percent of N-linked sites cleaved by endoglycosidase D or H. Thus the "fully deglycosylated" protein still contains N-acetyl glucosamine and fucose additions.

#The correlation between overall physical characteristics of a precipitate in a crystallization trial and the actual crystallization probability are imprecise. As a consequence, the comments made here describing precipitates are extremely qualitative. "Bad precipitates" indicate that most of the precipitates were yellow to light-yellow in color, indicative of denatured protein. "Good precipitates" indicates that in some conditions, the precipitates appeared to be microcrystalline, but individual crystals could not be discerned. "Ok precipitates" span the continuum between these two extremes.

Table 5. Crystallization conditions for initial gp120 crystals.

Crystal Type	Protein†	Concentration§	Reservoir Solution¶
A	ΔV1/2ΔV3 D1D2 sCD4	14.0	30% PEG 400, 0.2 M $MgCl_2$, 0.1 M Na Hepes pH 7.5 (reagent 23)
B	ΔV1/2ΔV3 D1D2 sCD4 Fab C11	9.2	2 M $(NH_4)_2SO_4$, 2% PEG 400, 50 mM $MgCl_2$ 50 mM Tris pH 8.5
C	ΔV1/2ΔV3ΔC5 D1D2 sCD4	11.0	6.7% PEG 4000, 3.3% isopropanol, 33 mM Na Hepes pH 7.5 (3-fold dilution of reagent 41)
D	Δ82ΔV1/2*ΔV3ΔC5 D1D2 sCD4 Fab 17b	7.6	15% PEG 4000, 0.1 M NH_4Acetate 50 mM NaCitrate pH 5.6 (2-fold dilution of reagent 9)
E	Δ82ΔV1/2*ΔV3ΔC5 D1D2 sCD4 Fab 17b	7.6	10% PEG 4000, 10% isopropanol 50 mM NaCitrate pH 5.6 (2-fold dilution of reagent 40)
F	Δ82ΔV1/2*ΔV3ΔC5 D1D2 sCD4 Fab 17b	6.6	6.7% PEG 8000, 15% isopropanol, 67mM $MgCl_2$ 33 mM Na Cacodylate pH 6.5 (3-fold dilution of reagent 18)

†All binary and ternary complexes were purified by gel filtration. D1D2 sCD4 refers to the two domain soluble CD4.

§The protein concentration is given as the absorbance (280 nm) of the complex per ml of solution.

¶Most of the reservoirs are conditions from Crystal Screen 1 (Hampton Research); the reagent numbers given here refer to the crystallization reagent from this commercial kit. Hanging droplets were 0.5 µl protein (in 0.35 M NaCl, 5 mM Tris pH 7.0, 0.02% NaN_3) + 0.5 µl reservoir, except for crystal type B, which used 0.5 ul of 3-fold diluted reservoir. Crystallization reservoirs were 500 µl; an additional 35 ul of 5 M NaCl was added after the droplet was mixed to compensate for the NaCl in the protein solution. All dilutions used H_20, except for crystal type F, where 22.5% isopropanol was used. Crystallizations were setup at room temperature and incubated at 20°C.

Table 6. Data collection statistics for Type E crystals of the two-domain CD4 (D1D2)/ Fab 17b / Δ82ΔV1/2*ΔV3ΔC5 gp120 complex.

	d_{range} (Å)	# reflections (unique)	R sym (%)	Completeness (%)
all data	20-2.2	56,195	14.5	87.4
last shell	2.48-2.2	13,928	35.5	73.1

TABLE 7

PROTEIN*	CONC	RESERVOIR SOLUTION**	µlP	µlR	FIGURE
A	11.0	Factorial 1 #40 500µl factorial/ 880µl Total vol. (1.76 dilution)	0.5	0.35	5 A,B
		Factorial 1 #28 500µl factorial/1375µl Total vol. (2.75 dilution)	0.5	0.35	6
	*	Factorial 1 #18 500µl/1375 total volume (2.75 dilution)	0.5	0.35	7
		Factorial 1 #14 +50µl 100% PEG 400 500µl/550µl total volume (50µl of PEG only)	0.5	0.35	8
		Factorial 1 #43 + 200µl Saturated AM_2SO_4 500µl only/700 µl total vol.	0.5	0.35	9
		PS Factorial #46 200µ factorial/ 600µl total volume	0.5	0.35	10
		PS Factorial #31 200µl factorial/ 550µl total volume (2.75 dilution)	0.5	0.5	11
		Factorial 1 #18 +50µl pH 4.5 Na Acetate 0.5M / 250µl factorial/ 688 total volume	0.5	0.35	12
B	5.2	PS Factorial #26 200µl factorial/ 800µl total volume (4.0 dilution)	0.5	0.5	13
		PS Factorial #28 200µl factorial/ 400µl total volume (2.0 dilution)	0.5	0.5	14

G	1.36	PS Factorial #35 200µl factorial/ 700µl total volume	0.5	0.5	15
M	1.4	PS Factorial #9 200µl factorial/ 200µl total volume	0.5	0.5	16
		Factorial 1 #32 500µl factorial/ 900µl total volume	0.5	0.35	17
N	6.2	Factorial 1 #17 500µl factorial/ 1300µl total volume	0.5	0.35	18
		Factorial 1 #18 500µl factorial/ 1300µl total volume	0.5	0.35	19
		Factorial 1 #38 500µl factorial/ 1000µl total volume	0.5	0.35	20
		* Factorial 1 #40 500µl factorial/ 1200µl total volume	0.5	0.35	21
		Factorial 1 #46 500µl factorial/ 900µl total volume	0.5	0.35	22
		PS Factorial #12 200µl factorial/ 300µl total volume	.05	0.5	23
		PS Factorial #29 200µl factorial/ 500µl total volume	.05	0.5	24
		Factorial 1 #40 + Factorial 1 # 16 150µl #16 250µl #40/600µl total vol.	0.5	0.35	25

* Crystals gave good diffraction

**NOTE: To all reservoirs 5M NaCl was added to bring the final concentration to 350mM. after droplet set up.

The final volume was made up by water, if there is a volume discrepancy.

+: **PROTEIN**

FAB/CD4/ISOLATE (DISTINGUISH gp120); CONSTRUCT NAME

A	$17b/D_1D_2/YU2(\Delta 82HYB.);\ \Delta 82\Delta V,_2{*}\Delta V_3\Delta C5$
B	$SC17b/D_1D_2/HxBC2(\Delta 82HYB);\Delta 82V_{1,2}{*}\Delta V_3\Delta C5$
G	$17b/D_1D_2/HxBC2(+V_3);\Delta 82\Delta V_{1,2}{*}\Delta C5$
M	$17b/D_1D_2/HxBC2(+C1C5HYB.);\Delta V_{1,2}{*}\Delta V_3$
N	$48D/D_1D_2/HxBC2(+C1C5HYB.);\Delta V_{1,2}{*}\Delta V_3$

++:

Factorial 1. is obtained in "Crystal Screen" provided by the Hampton Research, 27632 El Lazo Road, Suite 100, Laguna, Niguel, CA 92677- 3913, United States of America

PS FACTORIAL

F	% OF	ADDITIVE	PRECIPITANT	PH	SALT	ADDITIVE
9	5%	Isoproponal	4M NaCl		7.5	100mM $CaCl_2$
12	2%	PEG 400	2.5M Na/KPO_4	6.5		
26	10%	Isoproponal	30% PEG 1500	6.5	100mM	$CaCl_2$
28	8%	MPD	30% PEG 1500	8.5		
29	15%	Isoproponal	25% PEG 3,350		4.5	200mM AmCitrate
31	15%	MPD	25% PEG 3,350		6.5	200mM $LiSO_4$
35	10%	Isoproponal	20% PEG 8000	7.5	200mM	Am_4SO_4 ($(NH_4)_2SO_4$)
46	20%	PEG 1000	40% PEG 400	6.5	200mM	Na/KPO_4

MPD IS 2-METHYL-2,4-PENTANEDIOL; Am = NH_4

Second Series of Experiments

The human immunodeficiency viruses (HIV-1 and HIV-2) and simian immunodeficiency viruses (SIVs) are the etiologic agents of acquired immunodeficiency syndrome (AIDS) in their respective human and simian host (1). Typically, infection with primate immunodeficiency viruses is characterized by an initial phase of high-level viremia, followed by a long period of persistent virus replication at a lower level (2). Viral persistence occurs despite specific antiviral immune responses, which include the generation of neutralizing antibodies.

The primate immunodeficiency viruses, like all retroviruses, are surrounded by an envelope consisting of a host cell-derived lipid bilayer and virus-encoded envelope glycoproteins (3). For the virus to enter target cells, the viral membrane must be fused with the plasma membrane of the cell, a process mediated by the envelope glycoproteins. The exposed location of these proteins on the virus allows them to carry out their function but also renders them uniquely accessible to neutralizing antibodies. Thus, dual selective forces, virus replication and immune pressure, have shaped the evolution of the envelope glycoproteins and continue to do so within each infected host. Below summarized the current understanding of the functional features of these proteins.

<u>Synthesis and assembly of the envelope glycoproteins.</u> In the infected cell, the envelope glycoproteins are synthesized as approximately 845-870 amino acid precursor in the rough endoplasmic reticulum. (N)-linked, high-mannose sugar chains are added to form the gp160 glycoprotein, which assembles into oligomers (4-6). The preponderance of evidence suggests that these oligomeric complexes are trimers (4,5). The gp160

trimers are transported to the Golgi apparatus, where cleavage by a cellular protease generates mature envelope glycoproteins: gp120, the exterior envelope glycoprotein, and gp41, the transmembrane glycoprotein (3). The gp41 glycoprotein possesses an ectodomain that is largely responsible for trimerization (7), a membrane-spanning anchor, and a long cytoplasmic tail. Most of the surface-exposed elements of the mature, oligomeric envelope glycoprotein complex are contained on the gp120 glycoprotein. Selected, presumably well-exposed, carbohydrates on the gp120 glycoprotein are modified in the Golgi apparatus by the addition of complex sugar (6). The gp120 and gp41 glycoproteins are maintained in the assembled trimer by non-covalent, somewhat labile interactions between the gp41 ectodomain and discontinuous structures composed of N- and C-terminal gp120 sequences (8). Upon reaching the infected cell surface, a fraction of these envelope glycoproteins complexes are incorporated into budding virus particles. A large number of the complexes disassemble, releasing gp120 and exposing the previously buried gp41 ectodomain. These events contribute tot he formation of defective virions, which predominate in any retroviral preparation (9).

<u>Binding of the envelope glycoproteins to the CD4 receptor.</u>

Many cell surface proteins, including adhesion molecules, are incorporated into HIV-1 virions along with the envelope glycoprotein complexes (10). These host cell-derived molecules can assist the attachment of viruses to potential target cells. Virus attachment also involves the interaction of the gp120 envelope glycoproteins with specific receptors, the CD4 glycoprotein (11) and members of the chemokine receptor family (12, 13) (Fig. 26). The CD4 glycoprotein is expressed on the surface of T lymphocytes, monocytes,

dendritic cells, and brain microglia, the main target cells for primate immunodeficiency virus in vivo. The requirement for CD4 binding exhibited by most primate immunodeficiency viruses for efficient entry is consistent with this observed in vivo tropism. A major function of CD4 binding is to induce conformational changes in the gp120 glycoprotein that contribute to the formation and/or exposure of the binding site for the chemokine receptor (13, 14). Some HIV-1 and HIV-2 isolates cultured in the laboratory, as well as several primary SIV isolates, no longer depend upon CD4 for efficient entry, and bind to chemokine receptors but not CD4 for interaction (15). These examples and the observation that feline immunodeficiency viruses use chemokine receptors but not CD4 for entry (16) raise the distinct possibility that the chemokine receptors represent the primordial, obligate receptors for this retroviral lineage. The use of CD4 as a receptor may have evolved subsequently, allowing the high-affinity chemokine receptor-binding site of primate immunodeficiency viruses to be sequestered from host immune surveillance.

Multiple approaches have yielded insights into the structural basis for CD4-binding by the primate immunodeficiency virus gp120 glycoproteins. Early comparisons of gp120 sequences revealed the existence of five variable (V1-V5) regions interspersed with five conserved regions (17). Intramolecular disulfide bonds in the gp120 glycoprotein result in the incorporation of the first four variable regions into large, loop-like structures (6). Antibody binding studies and deletion mutagenesis have indicated that the major variable loops are well-exposed on the surface of the gp120 glycoprotein (18, 19). The more conserved regions fold into a gp120 core which has been recently crystallized in a complex with fragments of CD4 and a neutralizing

antibody (20). The gp120 core is composed of two domains, an inner domain and an outer domain, and a β sheet (the "bridging sheet") that does not properly belong to either domain (Fig. 27a). These names reflect the likely orientation of gp120 in the assembled envelope glycoprotein trimer: the inner domain faces the trimer axis and, presumably, gp41, while the outer domain is mostly exposed on the surface of the trimer. Elements of both domains contribute to CD4 binding. CD4 binds in a recessed pocket on gp120, making extensive contact over approximately 800 A$^{\circ 2}$ of the gp120 surface. Two cavities are evident in the gp120-CD4 interface. A shallow cavity is filled with water molecules, while a deep cavity extends 10-15 A$^{\circ}$ into the interior of gp120. The opening of this deep cavity is occupied by phenylalanine 43 of CD4, which has been shown by mutagenic analysis to be critical for gp120 binding (21). Most of the gp120 residues previously identified as important for CD4 binding (22,23) surround the opening of the deep cavity and contribute to interactions with phenylalanine 43 of CD4. In addition, aspartic acid 368 of gp120 forms a salt bridge with arginine 59 of CD4, also shown by mutagenesis to be important for gp120 binding (21). Additionally, mainchain atoms on gp120 and CD4 form hydrogen bonds bridging the two proteins. The formation of the deep cavity in gp120 likely contributes to the transmission of CD4-induced conformational changes to gp120 elements involved in the interaction with chemokine receptors and/or gp41. The deep cavity may be a useful target for intervention by small molecular weight compounds.

<u>Chemokine receptor binding</u>

Most primary, clinical isolate of primate immunodeficiency viruses use the chemokine receptors CCR5 for entry (12). For most HIV-1 isolated that are transmitted and that predominate during the early years

of infection, CCR5 is an obligate coreceptor, and rare individuals that are genetically deficient in CCR5 expression are relatively resistant to HIV-1 infection (24). HIV-1 isolates arising later in the course of infection often-use other chemokine receptors, frequently CXCR4, in addition to CCR5 (12,24). Studies of chimeric envelope glycoproteins demonstrated that the third variable (V3) loop of gp120 is a major determinant of chemokine receptor choice (12,25). V3-deleted versions of gp120 do not bind CCR5, even though CD4 binding occurs at wild-type levels (14). Antibodies against the V3 loop interfere with gp120-CCR5 binding (14). These results support an involvement of the V3 loop in chemokine receptor binding. Other, conserved gp120 structures also appear to play an important role in chemokine receptor binding. The use of CCR5 by a diverse group of immunodeficiency viruses with divergent V3 sequences, first suggest the involvement of more conserved gp120 elements (26). Antibodies that recognize conserved, discontinuous gp120 epitopes that are more exposed after CD4 binding are potent inhibitors of gp120-CCR5 interaction (14). These CD4-induced (CD4i) epitopes are discussed further below. Recent mutagenic and structural analysis have revealed the existence of a highly conserved gp120 structure that is important for CCR5 binding (20,27) (Fig. 27, a and b). This structure is adjacent to the V3 loop and the CD4i epitopes, and is oriented to face the target cell upon gp120-CD4 binding.

gp41-mediated membrane fusion.

It is likely that the interaction of the gp120-CD4 complex with the appropriate chemokine receptor promotes additional conformational changes in the envelope glycoprotein complex. By analogy with the influenza hemagglutinin, it has been suggested that the HIV-1 gp41 ectodomain undergoes major conformational changes during

virus entry (28). The proposed result of these changes is the insertion of the hydrophobic gp41 amino terminus (the "fusion peptide") into the membrane of the target cell. Mutagenic analysis (23,29) and the recently determined crystal structures of HIV-1 gp41 ectodomain fragments (5) are consistent with this model. The gp41 ectodomain structures reveal an extended, trimeric coiled coil that could potentially bridge the viral and target cell membranes (5). Interactions of other gp41 helical segments near the membrane-spanning region with the interhelical grooves of the internal coiled coil are important for fusion-related conformational changes in gp41. This interaction can be inhibited by helical peptides that mimic either of the involved gp41 helices (30) and is a potential target for future intervention with small molecular weight compounds.

The HIV-1 envelope glycoproteins as antigens.
The exposure of the primate immunodeficiency virus envelope glycoproteins on the surface of virions or infected cells makes them prime targets for antibodies that potentially block key functions of these proteins. However, the success of these viruses in achieving persistent infections implies that the viral envelope glycoproteins have evolved to be less-than-ideal immunogens and antigens. Structures on the viral envelope glycoproteins that are conserved among diverse viral strains are, in general, poorly exposed to the humoral immune system. The conserved gp120 surfaces involved in binding to its three minimally polymorphic ligands, gp41, CD4 and chemokine receptors, each exhibit particular problems with respect to the elicitation of sensitivity to neutralizing antibodies. The moieties involved in gp120-gp41 association are buried in the interior of the functional envelope glycoprotein spike (18, 31, 32). The CD4 binding sites is recessed, flanked by variable regions exhibiting considerable

glycosylation (19,20). The chemokine receptor-binding site is masked by variable loops, probably V3 and V2 (20,32,33) (Figure 27c). Even in the relatively conserved HIV-1 gp120 core that has been structurally analyzed, the outer domain exhibits a variable, heavily glycosylation surface (20). Since most carbohydrate moieties may appear as "self" to the immune system, this concentrated glycosylation may reduce the potential of a large portion of the gp120 surface to serve as an immunogenic target. Thus, in addition to the neutralizing and nonneutralizing faces of gp120 previously detected by antibody competition analysis (32), the crystal structure of the gp120 core reveals a third, immunologically silent face of gp120 (Fig 6D).

Despite the potential to exert potent antiviral effects, antibodies are not able to suppress virus replication completely in infected hosts. The efficacy of the humoral immune response in limiting virus spread in vivo is compromised by at least two factors: 1) the relative resistance of primary virus isolates to neutralization; and 2) the temporal pattern with which neutralizing antibodies are generated.

<u>Decreased neutralization sensitivity of primary HIV-1 isolates.</u>

HIV-1 viruses that have been passaged in immortalized cell lines are typically more sensitive to neutralization by antibodies or soluble CD4 than are primary, clinical isolates (34). Although other envelope glycoprotein regions can influence this phenotype, a major determinant is the structure of the gp120 major variable loops, V1/V2 and V3 (35). Thus, replacement of the V1/V2 and V3 variable loops of a laboratory-adapted virus with those of a neutralization-resistant primary isolate creates a virus similar to the parental primary virus (35). The basis for the

decreased sensitivity of primary HIV-1 isolates to neutralization appears to involve a decreased exposure of the relevant gp120 epitopes to soluble CD4 or antibody. This decrease is most apparent in the context of the assembled oligomeric complex (36). A likely explanation for this neutralization resistance is that the major variable loops of primary viruses assume tightly interfacing, "closed" conformations that decrease the accessibility of many gp120 epitopes to antibodies.

<u>The temporal pattern of the antibody response to HIV-1 infection.</u>

The noncovalent nature of the association between gp120 and gp41 contributes to the lability of the functional envelope glycoprotein trimer (8,9). During natural infections, disassembled envelope glycoproteins apparently elicit most of the antibodies directed against these viral components. The interactive regions of gp120 and gp41 are particular immunogenic (37). However, since the cognate antibodies cannot bind the assembled, functional envelope glycoprotein complex, they do not exhibit neutralizing activity. Thus, although antibodies against the envelope glycoproteins typically can be detected in the sera of HIV-1-infected individuals by two-three weeks after infection, most of these antibodies lack the ability to inhibit virus infection. By the time that neutralization antibodies are efficiently elicited, HIV-1 is firmly established in the host.

Several weeks after virus infection, usually after the initial high level of viremia has subsided, neutralizing antibodies can be detected in the sera of infected animals or humans (38). These antibodies neutralize the infecting virus but often exhibit little of no activity against other stains of virus. A subset of these

strain-restricted antibodies recognize the HIV-1 V3 loop (38). These antibodies can block chemokine receptor binding (14). Other variable gp120 elements can contribute to the epitopes recognized by the strain-restricted neutralizing antibodies. It is known, for example, that antibodies directed against the gp120 V2 loop can also exhibit neutralizing activity (39). The V2 loop-associated neutralization epitopes are typically conformation-dependent. The ability of some V2-or V3-directed antibodies to recognize more than one HIV-1 strain (39,40) suggests that these major variable loops assume a finite number of conformations. This is consistent with the functional consequences on virus entry of some changes in these variable structures (41), and with the observation that amino acid substitutions in the variable loops are not random (42). The requirement for chemokine receptor binding probably constrains V3 loop variation. The V2 loop, although dispensible for the replication of some HIV-1 viruses in culture (33), helps protect the V3 loop and the conserved epitopes near the chemokine receptor binding site from neutralizing antibodies. Thus, the V2 and V3 loops reside proximal to the chemokine receptor binding site (Fig. 27), masking more conserved gp120 elements and presenting potentially variable epitopes to the immune system.

Later in the course of HIV-1 infection of humans, antibodies capable of neutralizing a wider range of HIV-1 isolated appear (43). A subset of the broadly reactive neutralizing antibodies, found in most HIV-1 infected individuals, interferes with the binding of gp120 and CD4 (43). Human monoclonal antibodies derived from HIV-1 infected individuals have been identified that recognize the gp120 glycoproteins from a diverse range of HIV-1 isolates, that block gp120-CD4 binding, and that neutralize virus infection (44). The

discontinuous epitopes (the so-called CD4BS epitopes) recognized by many of these human monoclonal antibodies have been characterized by mutagenic analysis (45). The gp120 residues important for antibody binding are all located within the CD4-binding pocket on gp120 (Fig. 27b), and several of the most important residues are near the opening of the deep cavity (20). Therefore, some broadly neutralizing antibodies can apparently access the more recessed elements of the CD4 binding pocket. This is consistent with the observation that the gp120-CD4 interface is as large as that of a typical antibody-antigen complex (20).

A second group of neutralizing antibodies found in a smaller number of HIV-1-infected humans is directed against the CD4-induced (CD4i) epitopes (46). The CD4i epitopes are located near conserved gp120 structures important for chemokine receptor interaction (14) (Fig. 27b). CD4 binding has been shown to cause a change in the V2 loop conformation that allows better CD4i epitope exposure (33). In the absence of CD4, the antibodies recognizing the CD4i epitopes must bypass the overlapping V2 and V3 loops (33). Indeed, as is evident in the current crystal structure (20), this is accomplished by the protrusion of the CDR3 loop of the antibody heavy chain. Antibodies against CD4i epitopes need to bind viruses before CD4 binding occurs to achieve neutralization (47). The reason is that once the envelope glycoprotein complex binds cell surface CD4, there are severe steric constraints on the binding of an antibody to the gp120 surface facing the target cell (Fig. 26).

Another fairly conserved gp120 neutralization epitope is recognized by the 2G12 antibody (48). Unlike the other characterized HIV-1 neutralizing antibodies, which recognize gp120 structures near or within the receptor-

binding sites, the 2G12 antibody apparently binds an epitope in the outer domain (Fig. 27b). Given the variability in this outer domain, the ability of the 2G12 antibody to neutralize a fair number of HIV-1 strains (48) seems paradoxical. The marked sensitivity of 2G12 binding to alterations in gp120 glycosylation provides a clue to this puzzle. Despite the variability of the underlying primary amino acid sequence, the 2G12 antibody may recognize more conserved carbohydrate structures formed as a result of the heavy concentration of N-linked glycosylation in the gp120 outer domain. The apparent rarity with which 2G12-like antibodies are elicited attests to the success of the viral strategy of employing a heavily glycosylated outer domain surface in immune evasion.

<u>The HIV-1 envelope glycoproteins as vaccine components.</u> That the human and simian immunodeficiency virus envelope glycoproteins are not ideal immunogens is an expected consequence of the immunological selective forces that drove the evolution of these viruses. The same features of the envelope glycoproteins that dictate poor immunogenicity in natural infections have hampered vaccine development. The lability of envelope glycoprotein complex has frustrated attempts to present oligomers mimicking the functional spike to the immune system. As discussed above, the disintegration of envelope glycoprotein oligomers contributes to the preferential elicitation of non-neutralizing antibodies by the newly exposed gp120 N- and C-termini. Regardless of the context in which the envelope glycoproteins are presented, the gp120 variable loops elicit the majority of neutralizing antibodies, probably due to the exposed nature of these epitopes. It is still unclear whether conserved features in the V2 and V3 variable loops exist that can be exploited in vaccine design, or whether all possible functional configurations of these variable

structures need to be represented in a cocktail of immunogens.

The discontinuous gp120 structures surrounding the receptor binding sites exhibit a relatively high degree of conservation (20), in keeping with the minimal polymorphism in the host cell receptors. The CD4 binding site contributes a particularly attractive target. It appears to be accessible to antibodies, more so than the conserved elements of the chemokine receptor-binding region. A large fraction of the broadly neutralizing antibodies that eventually appear in HIV-1-infected individuals is directed against the CD4 binding site (43), indicating that ability of the human immune system to recognize this gp120 region and to generate an appropriate response. Nonetheless, these antibodies have been difficult to elicit in animals and vaccinated humans (49). The reasons for the relatively poor immunogenicity of the CD4 binding site are not yet understood, although several possibilities can be envisioned. Interdomain flexibility may disrupt the CD4BS epitopes and decrease their representation in the pool of immunogens. Masking by variable loops (19,33) and glycosylation may contribute to the recessed nature of the CD4BS epitopes which, even on the crystallized gp120 core, occupy a 20 A° deep canyon (20). Within the CD4-binding pocket, not all of the gp120 surface is conserved among HIV-1 strains. Therefore, even when elicited, some CD4BS-directed antibodies may lack the breadth and affinity to be optimal neutralization agents. While many monoclonal antibodies against the CD4 binding site exhibit reasonable potency and breadth (44), whether a polyclonal response against the envelope glycoprotein can be focused to preferentially contain these types of antibodies remains to be seen.

The conserved element near the chemokine receptor-

binding site will be difficult target for vaccine-elicited antibodies. Known monoclonal antibodies to the CD4i epitopes must interact with virus prior to CD4 binding if neutralization is to be achieved (47). Yet these gp120 structures are poorly exposed in the absence of CD4, in large part due the overlying V2 loop (33). This is consistent with the relative rarity with which these antibodies appear to be elicited in HIV-1-infected humans (46). Attempts to expose these structures better on gp120-based antigens seem warranted.

<u>Summary</u>

The HIV-1 envelope glycoproteins have evolved to be inefficient at eliciting effective antiviral antibody responses. The availability of structural information on the conserved HIV-1 gp120 neutralization epitopes should facilitate the modification of this important antigen and allow the rational testing of hypotheses regarding its poor immunogenic properties. These efforts should complement ongoing efforts to improve antigen presentation to the immune system and to create suitable animal models for the screening of vaccine candidates.

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Third Series of Experiments

The entry of human immunodeficiency virus (HIV) into cells requires sequential interactions of the viral exterior envelope glycoprotein, gp120, with the CD4 glycoprotein and a chemokine receptor on the cell surface. These interactions initiate a fusion of the viral and cellular membranes. Although gp120 can elicit virus-neutralizing antibodies, HIV eludes the immune system. We have solved the X-ray crystal structure at 2.5ů resolution of an HIV-1 gp120 core complexed with a two-domain fragment of human CD4 and an antigen-binding fragment of a neutralizing antibody that blocks chemokine-receptor binding. The structure reveals a cavity-laden CD4-gp120 interface, a conserved binding site for the chemokine receptor, evidence for conformational change upon CD4 binding, the nature of a CD4-induced antibody epitope, and specific mechanisms for immune evasion. Our results provide a framework for understanding the complex biology of HIV entry into cells and will guide efforts to intervene.

Introduction

Human immunodeficiency viruses, HIV-1 and HIV-2, and the related simian immunodeficiency viruses (SIV) cause the destruction of CD4+ lymphocytes in their respective hosts, resulting in the development of acquired immunodeficiency syndrome (AIDS)(1, 2). The entry of HIV into host cells is mediated by the viral envelope glycoproteins, which are organized into oligomeric, probably trimeric, spikes displayed sparsely on the surface of the virion. These envelope complexes are anchored in the viral membrane by the gp41 transmembrane envelope glycoprotein. The surface of the spike is composed primarily of the exterior envelope glycoprotein, gp120, associated by noncovalent

interactions with each subunit of the trimeric gp41 glycoprotein complex(3, 4.) When the gp120 sequences of different primate immunodeficiency viruses were initially compared, five variable regions (V1-V5) were identified (5). The first four variable regions form surface-exposed loops that contain disulfide bonds at their bases (6). The conserved gp120 regions form discontinuous structures important for the interaction with the gp41 ectodomain and with the viral receptors on the target cell. Both conserved and variable gp120 regions are extensively glycosylated(6). The variability and glycosylation of the gp120 surface likely modulate the immunogenicity and antigenicity of the gp120 glycoprotein, which is the major target for neutralizing antibodies elicited during natural infection (7).

Entry of primate immunodeficiency viruses into the host cell involves the binding of the gp120 envelope glycoprotein to the CD4 glycoprotein, which serves as the primary receptor. The gp120 glycoprotein binds to the most amino-terminal of the four immunoglobulin-like domains of CD4. Structures of both the N-terminal two domains (8, 9) and the entire extracellular portion of CD410 have been determined, and mutagenesis studies indicate that the CD4 structure analogous to the second complementarity-determining region (CDR2) of immunoglobulins is critical for gp120 binding(11, 12). Conserved gp120 residues important for CD4 binding have likewise been identified by mutagenesis (3, 13, 14).

CD4 binding induces conformational changes in the gp120 glycoprotein, some of which involve the exposure and/or formation of a binding site for specific chemokine receptors. These chemokine receptors, mainly CCR5 and CXCR4 for HIV, serve as obligate second receptors for virus entry (15, 16.) The gp120 third variable (V3) loop is the major determinant of chemokine receptor

specificity (17). However, other more conserved gp120 structures that are exposed upon engagement of CD4 also appear to be involved in chemokine-receptor binding. This CD4-induced exposure is indicated by the enhanced binding of several gp120 antibodies (18, 19) which, like V3-loop antibodies, efficiently block the binding of gp120-CD4 complexes to the chemokine receptor (20). These are called the CD4-induced (CD4i) antibodies. CD4 binding may trigger additional conformational changes in the envelope glycoproteins. For example, the binding of CD4 to the envelope glycoproteins of some HIV-1 isolates induces the release or "shedding" of the gp120 protein from the complex (21), although the relevance of this process to HIV entry is uncertain.

HIV and related retroviruses belong to a class of enveloped fusogenic viruses that includes corona-, paramyxo- and orthomyxoviruses (e.g. influenza virus), all of which require post-translational cleavage for activation. The transmembrane coat proteins of these viruses (gp41 equivalents) share sequence resemblance, particularly in their N-terminal fusion peptides, and they participate directly in membrane fusion. The ectodomain of gp41 can form a coiled coil resembling that of influenza hemagglutinin HA_2 (23, 4, 22,) supporting the notion that this class of viruses may share some common aspects with respect to virus entry. In other respects, enveloped viruses tend to be distinctive. They use varying modes of entry (direct membrane penetration for HIV, endocytosis for influenza virus) and even otherwise closely related viruses may use individualized receptors. The exterior coat proteins (gp120 equivalents) are accordingly specialized. Thus, for example, there is no detectable similarity in sequence, nor now in structure, between the receptor binding portion of HIV and that of murine leukemia virus (23), another retrovirus. Mechanisms for

receptor-mediated triggering of fusion may also be virus specific.

Because of the key role that the gp120 glycoprotein plays in receptor binding and in interactions with neutralizing antibodies, knowledge of the gp120 structure is important for understanding HIV infection and for the design of therapeutic and prophylactic strategies. Here, we report the crystal structure, at 2.5 A° resolution, of an HIV-1 gp120 core bound to a two-domain fragment of the CD4 cellular receptor and to the antigen-binding fragment (Fab) of an antibody, 17b, that is directed against a CD4i epitope. A companion report relates this structure to the antigenic properties of the gp120 envelope proteins(24).

Structure determination

The extensive glycosylation and conformational heterogeneity associated with the HIV-1 gp120 glycoprotein recommended a crystallization strategy aimed at radical modification of the protein surface. We made truncations at termini and variable loops in various combinations with gp120 from various strains, extensively deglycosylated these gp120 variants, and produced complexes with various ligands. A theoretical analysis showed that the probability of crystal formation is greatly increased by such reduction of surface heterogeneity and trials with multiple variants(25). After screening almost twenty combinations of gp120 variants and ligands, we obtained crystals of a ternary complex composed of a truncated form of gp120, the N-terminal two domains (D1D2) of CD4, and an Fab from the human neutralizing monoclonal antibody 17b (18, 25).

The crystallized gp120 is from the HXBc2 strain of

HIV-1. It has deletions of 52 and 19 residues from the N- and C- termini, respectively; Gly-Ala-Gly tripeptide substitutions for 67 V1/V2-loop residues and 32 V3-loop residues; and the removal of all sugar groups beyond the linkages between the two core N-acetylglucosamine residues. This deglycosylated core gp120 eliminates over 90% of the carbohydrate but retains over 80% of the non-variable-loop protein. Its capacity to interact with CD4 and relevant antibodies is preserved at or near wild-type levels26. The crystals are of space group $P222_1$ (a=71.6, b=88.1, c=196.7A°) with one ternary complex and 60% solvent in the crystallographic asymmetric unit.

The ternary structure was solved by a combination of molecular replacement, isomorphous replacement, and density modification techniques. It has been refined to an R-value of 21.0% (5-2.5 A° data > 2σ, R-free=30.3%). The final model, composed of 7877 atoms comprises residues 90-396 and 410-492 of gp120 (excepting loop substitutions), residues 1-181 of CD4, and residues 1-213 of the light chain and 1-229 of the heavy chain of the 17b monoclonal antibody. In addition, 11 N-acetylglucosamine and 4 fucose residues, and 602 water molecules have been placed. The overall structure of the complex of gp120 with D1D2 of CD4 and Fab 17b is as depicted in Fig. 28.

Structure of gp120

The deglycosylated core of gp120 as dissected from the ternary complex approximates a prolate ellipsoid with dimensions of 50 x 50 x 25ü, although its overall profile is more heart-shaped than circular. Its backbone structure is shown in Figs. 29a & c in an orientation precisely perpendicular to that in Fig. 28 (Fig. 31e gives a mutually perpendicular view). This

core gp120 comprises 25 b strands, 5 a helices and 10 defined loop segments, all organized with the topology shown in Fig. 29b. Specific spans of structural elements are given in Fig. 29d. The structure confirms the chemically determined disulfide bridge assignments (6; Fig. 29c). The polypeptide chain of gp120 is folded into two major domains plus certain excursions that emanate from this body. The inner domain (inner with respect to the N- and C-termini) features a two-helix, two-strand bundle with a small five-stranded β-sandwich at its termini-proximal end and a projection at the distal end from which the V1/V2 stem emanates. The outer domain is a stacked double barrel that lies alongside the inner domain such that the outer barrel and inner bundle axes are approximately parallel.

The proximal barrel of the outer-domain stack is composed from a 6-stranded, mixed-directional β-sheet that is twisted to embrace helix $\alpha 2$ as a 7th barrel stave. The distal barrel of the stack is a 7-stranded antiparallel β barrel. The two barrels share one contiguous hydrophobic core, and the staves also continue from one barrel to the next except at the domain interface. This interruption is centered at a side between barrels where the chain enters the outer domain with loop λB insinuated as a tongue between strands $\beta 16$ and $\beta 23$. The extended segment just preceding λB is like an 8th stave of the distal barrel, but it is slightly out of reach for hydrogen bonding with its $\beta 16$ and $\beta 19$ neighbors. The chain returns to complete the inner domain after $\beta 24$.

The proximal end of the outer domain includes variable loops V4 and V5 and loops λD and λE, which are variable in sequence as well. Loop λC is also at this end, close in space to loop λA of the inner domain, although by topology it is at the other end of this domain. The

distal end does include the stem of the excised variable loop V3 and also an excursion via loop λF into a β hairpin, β20-β21, which in turn hydrogen bonds with the V1/V2 stem emanating from the inner domain. This completes an antiparallel, 4-stranded "bridging sheet" that stands as a peculiar minidomain in contact with, but distinct from, the inner and outer domains as well as the excised V1/V2 domain. This bridging sheet also participates in the separated interactions of gp120 with both CD4 and the 17b antibody (Fig. 28 and below). One further excursion from the body of the outer domain produces strand β15 and helix α3, which are also important in CD4 binding.

Taken as a whole the structure of gp120 seen here is novel. Moreover, our domain-level searches have failed to reveal similarity of the inner domain to any known atomic structures, although the missing terminal segments might conceal relationships. We do, however, find a fragmentary similarity for portions of the outer domain with known structures. In particular, part of the protomer of FabA dehydrase (27) is like part of the proximal barrel, and dUTP pyrophosphatase (28) has elements in common with both barrels of the outer domain. In each case the superimposable fraction is limited. For FabA, 45 of its 171 C-alpha atoms superimpose on five segments, but the rest are topologically unrelated. For dUTPase, 41 of its 152 C-alpha atoms appropriately capture 8 of the 15 segments in the outer domain body, but there is no helix corresponding to alpha-2 and the placements of termini are not comparable. Interestingly, several viruses related to HIV encode dUTPases; however, we have not found sequence evidence to support a possible role in coat protein evolution.

This structure of core gp120 should be a prototype for

the class. As shown in the structure-based alignment of representative sequences (Fig. 29d), there is substantial conservation despite the noted variability among HIV strains. Thus, even an HIV-2 sequence is 35% identical with that of the HXBc2 strain expressed in this crystallized construct, and the identity level rises to 77% and 51%, respectively, for the more closely related HIV-1 clade C and clade O representatives. The inner domain is appreciably more conserved than the outer domain with 86%, 72% and 45% identity for the respective C, O and HIV-2 comparisons. Variability correlates with the degree of solvent exposure of residues (Fig. 29d), in keeping with the conservation of hydrophobic cores. The seven disulfide bridges retained in core gp120 are absolutely conserved and mostly buried (Fig. 29c). Glycosylation sites are all surface exposed and are conserved above average (Fig. 29d). The previously identified HIV variable segments(5) are all on loops connecting elements of secondary structure, and loops λD and λE are also especially variable. Indeed, λE is more variable than V5 in light of current sequence data. These loops are also relatively mobile as reflected in high B factors or disorder, as in V4. Interestingly, variable segments in the outer domain, including the exposed face of α2, appear to arise from neutral mutation rather than selective pressure since they are on non-immunogenic surfaces, presumably masked by glycosylation.

CD4-gp120 interaction

CD4 is bound into a depression formed at the interface of the outer domain with the inner domain and the bridging sheet of gp120 (Figs. 30a). This interaction buries a total of 742 A^{o2} from CD4 and 802 A^{o2} from gp120. The surface areas that are actually in contact are considerably smaller (Fig. 30d) because an unusual

mismatch in surface topography creates large cavities that are occluded in the interface, as described below. There is, however, a general complementarity in electrostatic potential at the surfaces of contact, although the match is imprecise in this respect as well. The focus of CD4 positivity is displaced from the center of greatest negativity on gp120 (Fig. 30c). The binding site is devoid of carbohydrate (Fig. 30g). The structure of CD4 in this complex differs only locally from that in free D1D2 structures and at only a few places: residues 17-20 at the poorly ordered CDR1-like loop and residues 41,42,47,49 and 60, which are at or near the contact site and have low B factors in the gp120-bound state.

Direct interatomic contacts are made between 22 CD4 residues and 26 gp120 amino-acid residues. These include 219 van der Waals contacts and 12 hydrogen bonds. Residues in contact are concentrated in the span from 25 to 64 of CD4, but they are distributed over six segments of gp120 (Figs. 29d & 30i): 1 residue from the V1/V2 stem, loop LD, the beta-15-alpha-3 excursion, the beta-20-beta-21 hairpin, strand beta-23 and the beta-24-alpha-5 connection. These interactions are compatible with previous analyses of mutational data on both CD4(11, 12, 29) and gp120(3, 13, 14). Other groups are also involved, including some at gp120 sites that have not been tested, but residues identified as critical for binding do indeed interact with one another (Fig. 30e). Most importantly, Phe 43 and Arg 59 of CD4 make multiple contacts centered on residues Asp 368, Glu 370 and Trp 427 of gp120, which are all conserved among primate immunodeficiency viruses. In fact, 63% of all interatomic contacts come from one span (40-48) in C′C" of CD4, and Phe 43 alone accounts for 23% of the total. Similarly, with respect to gp120, the spans of 365-371 and 425-430 contribute 57% of the total. Of the three

CD4 lysine residues implicated in binding (residues 29, 35 & 46), only Lys 29 makes a direct ionic hydrogen bond, and while Asp 457 of gp120 is near to these electropositive groups (Figs. 30e & i) it does not make hydrogen bonds.

Several gp120 residues that are covered by CD4 are variable in sequence. This variation is accommodated in part by the large interfacial cavity (Fig. 30e). The gp120 residues in contact with this water-filled cavity are especially variable (Fig. 30g). Moreover, half of the gp120 residues that make contacts with CD4 do so only through main-chain atoms (including Cβ) of gp120, and 60% of CD4 contacts are made by gp120 main-chain atoms (Fig. 30f). Included among these are 5 of the 12 hydrogen bonds in the interface. One such contributing element is an antiparallel β-sheet alignment of CD4 strand C" with gp120 strand beta-15 (Figs. 30a & i).

Atomic details of the interaction are particularly intricate and unusual for the contacts made between gp120 and the mutationally critical CD4 residues Phe 43 and Arg 59 (Fig. 30j). Arg 59 interacts with Asp 368 and Val 430. The carboxylate group of Asp 368 makes double hydrogen bonds with the guanidinium Nη atoms of Arg 59, but it also hydrogen bonds back to the backbone NH group of residue 44 and it appears to be optimally positioned to receive a CH...O hydrogen bond (3.20 Å) from the Phe 43 ring. Phe 43 interacts with residues Glu 370, Ile 371, Asn 425, Met 426, Trp 427 and Gly 473 as well as Asp 368, but only the contacts with Ile 371 have a conventional hydrophobic character. Those to 425-427 and 473, including Trp 427, are only to backbone atoms. A surprisingly large fraction of the Phe 43 contacts (28%) are to polar groups. The phenyl group is stacked on the carboxylate group of Glu 370, and there are contacts with the carbonyl oxygen atoms of residues

425, 426 and 473 and the NH group of Trp 427. Indeed, at a distance of 3.10 Å, the phenyl contact with O 425 is a second candidate CH...O hydrogen bond. Asp 368 and Glu 370 have their carboxylate groups close together (3.54 Å) and they are, of course, buried in the complex. Even for gp120 excised from the complex, their fractional surface accessibilities are only 44% and 14%, respectively. Glu 370 may therefore be protonated. Perhaps the most extraordinary aspect of this site is the large cavity beyond Cζ of Phe 43 (Figs. 30b & h, and below).

Interfacial cavities

Analysis of the solvent accessible surface of the ternary complex reveals a number of topologically interior surfaces or cavities. Two of these, both at the gp120-CD4 interface, are unusually large. The larger (279 $Å^3$) is formed at the interface between the slightly concave middle of the CC'C" portion of the CD4 sheet, and a groove on gp120 where beta-23 and beta-24 are indented relative to beta-15 and the λD loop (Fig. 30e). The second is from a pocket in the gp120 surface that is plugged by Phe 43 from CD4 (152 $Å^3$). This pocket is itself at the interface between the inner and outer domains of gp120 (Fig. 30h). Several other smaller cavities are also wedged at the interface between the two gp120 domains.

The larger cavity is lined by mostly hydrophilic residues, half derived from gp120 and half from CD4. It is not deeply buried; while formally a cavity in the crystal structure, minor changes in sidechain orientation would make it solvent accessible. The observed electron density and predicted hydrogen bonding are consistent with at least 8 water molecules in the cavity. Residues from gp120 that actually line the

cavity (including Ala 281, Ser 364, Ser 365, Thr 455, Arg 469) exhibit sequence variability, whereas surrounding this variable patch are conserved residues, the substitution of which affect CD4 binding. These include the critical contact residues Asp 368, Glu 370 and Trp 427, which flank one end of the cavity, and Asp 457 at the other end (Fig. 30e). Similarly, CD4 residues that line the cavity (e.g., Gln 40 and Lys 35) can be mutated with only moderate effect on gp120 binding, whereas Arg 59 suffers less loss of solvent accessible surface upon gp120 binding but is highly sensitive to mutation. This cavity thus serves as a water buffer between gp120 and CD4 (Fig. 30e). The tolerance for variation in the gp120 surface associated with this cavity produces a variational island (Fig. 30g), or "anti-hot spot", which is centrally located between regions required for CD4 binding, and may help the virus escape from antibodies directed against the CD4 binding site.

The "Phe 43" cavity (Fig. 30b & h) is very different in character from the larger binding-interface cavity. It is roughly spherical, with a diameter of ~8 Å (atom center to atom center) across the center of the cavity. It is positioned just beyond Phe 43 of CD4, at the intersection of the inner domain, the outer domain and the bridging sheet. It is relatively deeply buried, extending into the hydrophobic interior of gp120. The phenyl ring of Phe 43 is the only non-gp120 residue contacting this cavity, forming a lid which covers the bottom of the cavity (Fig. 30b). Other routes of solvent access are possible: past Met 426 under the bridging sheet, or directly through the heart of gp120, at the inner domain-barrel domain interface. Ordered water molecules demarking possible paths of solvent access are found along both routes. Nonetheless, in the cavity itself, only a few water molecules are observed.

The center of the cavity is dominated by a large piece of spherical density, which is over 4 Å from any protein atom (Fig. 30b). The size, shape and predicted hydrogen bonding of this density is inconsistent with those expected for water, isopropanol, ethylene glycol, or any of the other major crystallization components. We have been unable to identify the source of this density.

Residues that line the Phe 43 cavity (side chains of Trp 112, Val 255, Thr 257, Glu 370, Phe 382, Tyr 384, Trp 427 and Met 475; main chains of 255-257 and 375-377) are primarily hydrophobic. They are also highly conserved, as much so as the buried gp120 hydrophobic core. Despite a lack of steric hindrance, almost no substitutions to larger residues are found. Given the frequency of gp120 sequence divergence, such conservation strongly implies functional significance. Indeed, although residues that line this cavity provide little direct contact to CD4, they do nevertheless affect the gp120-CD4 interaction. Thus, mutations at Thr 257 (no contacts) and Trp 427 (only main-chain contacts) can substantially reduce binding. Changes in cavity-lining residues also affect the binding of antibodies directed against the CD4 binding site. In addition, many of the residues that line the cavity interact with elements of the chemokine receptor binding region (see below). It may be that the Phe 43 cavity and the other interdomain cavities form as a consequence of a CD4-induced conformational change (see below).

Despite this unusual cavity-laden interface between gp120 and CD4 interface, we believe that this structure reflects the true character of the interaction. Core gp120 binds CD4 with essentially the same affinity(26) and residues identified as critical by mutational analysis on both components are indeed at the focus of contact in the structure. In any case, the missing

loops and termini could not conceivably have a role in filling these cavities.

Antibody interface

The 17b antibody is a broadly neutralizing human monoclonal isolated from the blood of an HIV-infected individual. It binds to a CD4-induced (CD4i) gp120 epitope that overlaps the chemokine receptor-binding site(20).

Relative to other antibody-antigen pairs (Fig. 31a-c), the interface between Fab 17b and core gp120 in the ternary complex involves a small area of interaction. The solvent accessible area excluded upon binding is only 455 Å^2 from gp120 and 445 $^2\text{Å}$ from 17b, which is largely from the heavy chain (371Å^2). The long (15 residue) complementarity-determining region 3 (CDR3) of the heavy chain dominates, but the heavy-chain CDR2 and the light-chain CDR3 also contribute. Overall, the 17b contact surface is very acidic (3 Asp, 3 Glu, no Arg or Lys) although hydrophobic contacts (notably a cis proline and tryptophan from the light chain) predominate at the center.

On gp120, the 17b epitope lies across the base of the four-stranded bridging sheet (Fig. 31c & e). All four strands make substantial contact with 17b, suggesting that the integrity of the bridging sheet is necessary for 17b binding. The gp120 surface that contacts 17b consists of a hydrophobic center surrounded by a highly basic periphery (3 Lys, 1 Arg, and no Asp or Glu) (Fig. 31d). Although this basic gp120 surface complements the acidic 17b surface, only one salt bridge is observed (between Arg 419 of gp120 and Glu 106 of the 17b heavy chain). The rest of the specific contacts occur between hydrophobic and polar residues. Thus, the interaction

between 17b and gp120 involves a hydrophobic central region flanked on the periphery by charged regions, predominately acidic on 17b and basic on gp120. There are no direct CD4-17b contacts and none of the gp120 residues contacts both 17b and CD4. Rather, CD4 binds on the opposite face of the bridging sheet, providing specific contacts that appear to stabilize its conformation (Fig. 30i and 30j) and may explain in part the CD4-induction of 17b binding.

The 17b epitope is well conserved among HIV-1 isolates. Of the 18 residues that show loss in solvent accessible surface upon contact with 17b, 12 residues (67%) are conserved among all HIV-1 viruses. By contrast, only 19 of the 37 gp120 residues (51%) that show loss of solvent accessible surface upon CD4 binding are similarly conserved. CD4i epitopes tend to be masked from immune surveillance by the adjacent V2 and V3 loops (see accompanying paper). Indeed, in the complex structure, a large gap is seen between gp120 and tips of the light-chain CDR1 and CDR2 loops. Pointing directly at this gap is the base of the V3 loop. In intact gp120, the variable loops may need to be bypassed for access to the conserved structures in the bridging sheet. The 17b epitope may be further protected from the immune system by a CD4-induced conformational change (see below).

Chemokine receptor site

The site of interaction with the chemokine receptor CCR5 overlaps with the 17b epitope(30). Both are induced upon CD4 binding and both involve highly conserved residues. By mutational analysis, the basic and polar gp120 residues (Lys 121, Arg 419, Lys 421, Gln 422) that contact the 17b heavy chain also are important for CCR5 interaction(30). The hydrophobic and acidic surface of the 17b heavy chain may mimic the tyrosine-rich, acidic

N-terminal region of CCR5, which is important for gp120 binding and HIV-1 entry (31, 32). Geometrically, this site is directed at the cellular membrane when gp120 is engaged by CD4. Electrostatic interactions between the basic surface of the bridging sheet and the acidic chemokine receptor (and possibly the acid headgroups in the target membrane) could drive conformational changes related to virus entry.

Oligomer and gp41 interactions

Although monomeric in isolation, gp120 likely exists as a trimeric complex with gp41 on the virion surface. The large electroneutral surface on the inner domain (Fig. 30c) is the probable site of trimer packing based on its lack of glycosylation, its conservation in sequence, the location of CD4 and CCR5 binding sites, and the immune response to this region. These points are elaborated in the accompanying paper and a model is presented(24).

A large body of mutagenic and antibody-binding analyses suggest that the N- and C-termini of full-length gp120 are the most important regions for interaction with the gp41 glycoprotein (33, 34). From these analyses, we expect that gp41 interactive regions will extend away from core gp120 toward the viral membrane, and that the conserved, electroneutral surface is occluded in the oligomer/gp41 interface. A similar arrangement is seen in influenza hemagglutinin, where the extended N- and C-termini of HA_1 interact with the HA_2 transmembrane protein (35).

Conformational change in core gp120

There is abundant evidence to suggest that CD4 binding induces a conformational change in gp120. Much of this evidence, however, derives from intact gp120 with

variable loops in place or from the oligomeric gp120:gp41 complex. The ternary complex structure provides clues to conformational changes within core gp120 itself. (Although 17b binding could contribute to the gp120 conformation observed in the crystal, the CD4 contacts are much more extensive and multifaceted than those of 17b. These observations argue that CD4 binding plays the major role in the formation of the observed gp120 structure.)

Were the conformation of gp120 seen here preserved in the absence of CD4, the Phe 43 cavity (now a pocket) would present a perplexing structural dilemma. As discussed above, the cavity-lining residues have few structural restrictions, with ample room for larger substitutions into the cavity, yet these residues are highly conserved and inexplicably hydrophobic if exposed in a pocket. This pocket structure is in turn intimately connected to the bridging sheet, itself peculiar in absence of CD4. Thus, for example, the backbone amide of bridging-sheet residue 425 is hydrogen-bonded to Glu 370, a critical CD4 contact residue (Fig. 30j); Ile 424 makes extensive hydrophobic contacts with Phe 382, which lines the pocket from the outer domain; and Trp 427 packs perpendicular to Trp 112, which lines the pocket from the inner domain (Fig. 30b). Nε of Trp 427 is delicately poised for hydrogen-bonding with the π-electrons of the indole ring of Trp 112. Structures such as these would necessarily be very sensitive to orientational shifts between the inner and outer domains.

The characteristics of 17b binding to core gp120 provide additional evidence for a CD4-induced conformational change. We do not observe detectable binding of Fab 17b to core gp120 unless CD4 is present, but then the ternary complex is stable in gel filtration. Since

there are no direct CD4-17b contacts in the structure, the effect of CD4 must be to stabilize the bridging-sheet minidomain to which 17b binds. This result is compatible with the binding properties of 17b and other CD4i antibodies to full-length gp120(18) (see accompanying paper), but it shows that the conformational change is not limited to an unmasking of the antibody epitope by CD4-induced of the V2 loop, as initially thought(36). The ability of the 17b antibody to bind full-length gp120 in the absence of CD4, albeit at a lower level, implies that structural elements required for 17b binding can be accessed in the absence of CD4. If we assume that 17b binds in the same way to both full-length and core gp120, as shown by the concordance between the structural contacts (Fig. 31) and epitope mapping data, this suggests that alternative conformations are in a kinetically accessible equilibrium in native gp120.

A further indication that core gp120 may differ in the absence of CD4 comes from comparison with theory. When applied to the many known sequence variants of gp120, the evolutionary algorithm of PHD37 gives secondary-structure predictions with 90% estimated reliability for roughly 45% of the core gp120 sequence. Compared to our structure, it is accurate except at three places where it is markedly wrong (four consecutive residues with reliability index greater than 90%). All of these are at the Phe 43 cavity or in contacts with CD4: loop λB, strand β15, and the segment of β20 into the turn to β21. (Fig. 30h). Most significantly, the latter segment (residues 422-429) entering the bridging sheet is predicted to be helical. Indeed, residues 427-428 at the β20-β21 turn do have helical character. We also note that CD4 binds efficiently to a gp120 derivative with both β2 and β3 truncated(38). Since the bridging sheet is most likely

not stable in the absence of half its strands, CD4 binding must possess the ability to properly orient strands $\beta 20$ and $\beta 21$ from a very different prior conformation.

The Phe 43 cavity is at the nexus of the CD4 interface, between the inner domain, the outer domain, and the bridging sheet. As such, Phe 43 itself seems to serve as a keystone without which the structure might collapse. If so, to what state and, in reverse, how does CD4 binding lead to the state seen in this ternary complex? Certainly, it is clear that CD4-gp120 binding kinetics are complex(39), and microcalorimetric analysis reveals unusually large ΔH and compensating $T\Delta S$ values for soluble CD4 binding to gp120 (M. L. Doyle, personal communication). These exceptional CD4-binding thermodynamics imply a large conformational change and are similar for both full-length and core gp120, which further supports the relevance of the structural observations on core gp120. We imagine that CD4 sees gp120 as an uneven equilibrium of conformational states, makes initial contact through electrostatic interactions (Fig. 30c), stabilizes a nascent complex state, and inserts the Phe 43 to induce formation of the Phe 43 cavity.

Viral evasion of immune surveillance

Analysis of the antigenic structure of gp120 shows that most of the envelope protein surface is hidden from humoral immune responses by glycosylation and oligomeric occlusion (accompanying paper). Most broadly neutralizing antibodies generally access only two surfaces, one which overlaps the CD4 binding site (shielded by the V1/V2 loop) and the other which overlaps the chemokine receptor binding site (shielded by the V3 loop). Conformational changes in core gp120

provide additional mechanisms for evasion from immune surveillance. In the case of the CD4-binding surface, which contains a high proportion of mainchain atoms in the complex (Fig. 30f), the conformation without CD4 bound may expose underlying sidechain variability (Fig. 30g). Escape may also be provided by the recessed nature of the binding pocket (steric occlusion) (Fig. 30a) and by a topographical surface mismatch, which encloses a variational island or "anti-hot spot" (described above, Fig. 30d). Similar mechanisms may be found in the chemokine receptor region: conformational change may hide the conserved epitope (unformed prior to CD4 binding); steric occlusion may take place between the CD4 anchored viral spike and the proximal target membrane; and an "anti-hot spot" equivalent may camouflage chemokine-receptor binding residues on the V3 loop in surrounding variability. Some of the defenses used to elude antibody-based responses may also help HIV avoid cellular immunity. Understanding the specific gp120 mechanisms of immune evasion may be prerequisite to the design of effective prophylaxis.

Mechanistic implications for virus entry

During virus entry, the HIV surface proteins function to fuse the viral membrane with the target cell membrane. The gp120 glycoprotein plays roles crucial to the control and initiation of fusion. One set of roles concerns positioning: locating a cell capable of productive viral infection, anchoring the virus to the cell surface, and orienting the viral spike next to the target membrane. Another set concerns timing: holding the gp41 in a metastable conformation and triggering the coordinate release of the three N-terminal fusion peptides of the trimeric gp41. While it is clear that this is a complex multi-conformational process, the simplicity of the system, composed only of two

membranes, the viral oligomer, and two host receptors, raises the possibility that we may be able to understand the entire mechanism. Crystallography has now provided two snapshots: an intermediate state in which gp120 is bound to CD4, described herein; and a probably final, "fusion-active" state of the gp41 ectodomain (40,41). Although precise structural information is lacking for other intermediates, the vast biochemical data concerning the membrane fusion process mediated by the HIV-1 envelope glycoproteins allow us to extend our understanding from these two states.

The entry process is initiated by the binding of HIV-1 to the cellular receptor CD4 (Fig. 32, step 1). Although the extracellular portion of CD4 has some segmental flexibility, this binding roughly orients the viral spike. This orientation can be simulated by an alignment of the D1D2 CD4 in the ternary complex with the previously solved structure of the four-domain, entire extracellular portion of CD4(10). Such alignment orients the N- and C- termini of core gp120 towards the viral membrane, while the 17b epitope/chemokine receptor-binding site on the gp120 surface faces the target cell membrane. Such an orientation is consistent with the proposed oligomeric structure and gp41-interactive surfaces described above.

CD4 binding also induces conformational changes in gp120, which result in the creation of a metastable oligomer. Although some of the more flexible gp120 regions and gp41 are missing, the structure of the core gp120-CD4 complex presented here describes this state in atomic detail. CD4 binding results in movement of the V2 loop, which numerous experiments suggest partially occludes the V3 loop and CD4i epitopes (18, 36). It also creates, or at least stabilizes, the bridging sheet on which these epitopes are located (described above for

the core). In addition, CD4 binding results in changes in the conformation of the V3 region, with the tip of the loop becoming more accessible, as judged by enhanced proteolytic susceptibility and altered exposure of V3 epitopes(19). The V3 loop together with the uncovered epitopes comprise the chemokine-receptor binding site. Thus, CD4 binding not only orients the gp120 surface implicated in chemokine receptor binding to face the target cell, but it also forms and exposes the site itself. We note that these changes may all result from a single, concerted shift in the relative orientation of the inner and outer domains. This conformational shift may alter the orientation of the N- and C- termini, at the proximal end of the inner domain, perhaps partially destabilizing the oligomeric gp120/gp41 interface(21). Such a shift would also alter the relative placement of the V1/V2 stem (in the CD4i site), which emanates from the inner domain, and the V3 loop, which emanates from the outer domain. Interestingly, mutations that permit an adaptation of HIV-1 to CD4-independent entry using CXCR4 involve sequence changes in both the V1/V2 stem and the V3 loop(42).

The next step in HIV-1 entry is the interaction of the gp120-CD4 complex with the chemokine receptor (Fig. 32, step 2). Although interactions between CD4 and chemokine receptor may occur, mutagenic analyses (H. Choe and J. Sodroski, unpublished observations) and the known examples of CD4-independent virus entry or chemokine-receptor binding suggest that direct gp120 contacts dominate in the interaction with the chemokine receptor. Since most of the chemokine receptor is encased in the host membrane, binding would necessarily move the gp120 bridging sheet close to the target membrane. This movement requires CD4 flexibility since the initial HIV binding at the N-terminal D1 domains probably occurs above the glycocalyx. Reducing

flexibility at the D2-D3 juncture or at the D4-membrane juncture of CD4 has been shown to block HIV-1 entry (10, 43).

Chemokine-receptor binding is believed to trigger additional conformational changes in the HIV-1 envelope glycoprotein trimer which lead to exposure of the gp41 ectodomain. Presumably, a signal is transmitted from the cell-associated distal end of gp120 to elements of the inner domain that are likely to be involved in gp120-gp41 or gp120-gp120 association on the trimer. Although further inter-domain shifts may occur in core gp120 after chemokine-receptor binding, the geometrically specific contacts that support the bridging sheet make it unlikely that another shift could occur without destabilizing this important component of the chemokine-receptor binding site. Since the high affinity of interaction makes it likely that both CD4 and chemokine receptor remain bound to gp120 during fusion, we expect that additional conformational changes probably occur between neighboring gp120 protomers in the oligomeric complex. Perhaps the chemokine receptor triggers gp41 exposure by prising gp120 protomers away from the trimer axis thus exerting a torque on the gp120-gp41 interface. In this regard it is interesting that several of the substitutions that affect chemokine-receptor binding in the context of monomeric gp120 appear to induce gp120 dissociation in an oligomeric context(30).

The structure of the gp120/CD4/17b antibody ternary complex described here reveals some of the molecular aspects of HIV-1 entry, including the atomic structure of gp120, the explicit interactions with CD4, and the conserved site of binding for the chemokine receptor. Still unknown are details of the apo state of core gp120, the oligomeric structure, the interaction with

the chemokine receptor, the conformational changes that trigger the reorganization of the gp41 ectodomain and the structural basis for insertion of the fusion peptide of gp41 into the target membrane. Further understanding will require snapshots of other intermediates. The conformational complexity and observed intricate domain associations of gp120, like those of reverse transcriptase(44), the other large HIV translation product, may reflect genome restrictions at the protein level akin to those that lead to overlapping reading frames at the transcription level. Multiply protected infection machinery is contained in these condensed intricacies. Its mechanisms frustrate host defenses; understanding them may inspire medical intervention.

Methods

Protein production, crystallization, and data collection. The two-domain CD4 (D1D2, residues 1-182) was produced in Chinese hamster ovarian cells(8), the monoclonal antibody 17b in an Epstein-Barr virus immortalized B-cell clone isolated from an HIV-1 infected individual and fused with a murine B-cell fusion partner(18), and the core gp120 from Drosophila Schneider 2 lines under control of an inducible metallothionein promoter (20). The various biochemical manipulations (e.g. deglycosylation for the gp120 and papain digestion to produced the Fab 17b), protein purification, and ternary complex crystallization are described elsewhere(25). The best crystals were small needles of cross-section only 30-40 μm. These were crosslinked with vapor diffusion glutaraldehyde treatment (C. J. Lusty, personal communication), equilibrated with cryoprotectant containing stabilizer (10% ethylene glycol with 10.5% monomethyl-PEG 5,000, 10% isopropanol, 50 mM NaCl, 100 mM Citrate/HEPES buffer pH 6.3), transferred into immiscible oil (Paratone-N;

Exxon), suspended in a small ethylene loop at the end of a mounting pin, and flash-frozen in a cryostat nitrogen stream at 100 K .

Diffraction data were collected at beamline X4A, Brookhaven National Laboratory, using phosphor image plates and a Fuji BAS2000 scanner. To avoid overlap problems from the relatively high mosaicity (~1.0°), oscillation data were collected using a rotation axis that was off-set at least 30° from the 197Å c axis. Although crystals initially diffracted to Bragg spacing of greater than 2Å, β axis mosaicity and substantial radiation damage despite cryogenic cooling reduced the overall resolution to ~2.5Å. Data processing and reduction were performed using DENZO and SCALEPACK(45) (Table 1).

Structure determination and refinement. To locate the position of the Fab 17b in the ternary complex crystals, rotational searches with 52 different Fab models were made with the program MERLOT (P. M. Fitzgerald). The Fabs were aligned by superposition of their variable domains to allow comparison of rotational solutions. Even though four models showed greater than 10% discrimination between highest and second highest solutions, no consistent rotational solution was found. Discrimination between correct and incorrect solutions was achieved by using confirmatory searches with the variable portion of the Fab. This was successful with only one model, molecule B of 1hil. Rigid body refinement of the 1hil solution (XPLOR(46)), allowing each immunoglobulin domain to move independently, produced a Patterson correlation of 24.9%. To locate the position of the two-domain CD4, each of the top 100 possible rotational solutions with each of three different CD4 models (1cdi, 1cdh, 3cd4), were searched for a distinctive translation solution (AMoRe; J.

Navaza). The translation searches used the rigid body refined Fab as a partial structure to help discriminate the correct solution. Two distinctive solutions were found: the 25th rotational solution of 3cd4 gave a translation correlation of 0.171 (verses 0.128 for the second highest translation solution), and the 61st rotational solution of 1cdh gave 0.149 (verses 0.140). These two solutions were virtually identical. Rigid body refinement in XPLOR(46) gave a Patterson correlation of 7.9% for the CD4 alone and 32.4% for the Fab and CD4. All molecular replacement and rigid body refinements used 8-4Å data.

To provide additional phasing, crystals were soaked in over 20 different heavy atom solutions and screened for isomorphous replacement using the statistical <chi>2 test in SCALEPACK(45). Derivatives were identified from two heavy atom compounds : 10 mM K_3IrCl_6 (10 hr equilibration in heavy atom containing cryoprotectant stabilizer; 2.8Å) and 5 mM K_2OsCl_6 (24 hr soak; 3.5Å). Isomorphism was found to be highest between these heavy atom data sets and a native data set collected at pH 7.0 (cryoprotectant stabilizer buffered with 50 mM BisTris pH 7.0). Heavy atom sites were identified by difference Fourier analysis using the molecular replacement phases, and phasing parameters were refined with MLPHARE (in the CCP4 suite of crystallographic programs). The K_3IrCl_6 derivative was modeled as 9 partially occupied sites; two sites of occupancy 0.158 and 0.142, and 7 of less than 0.07. While relatively isomorphous, poor data quality (Rsym of greater than 20% past 3.0Å) combined with relatively small isomorphous differences (Riso of 12.0%) reduced the quality of phasing. In contrast, the K_2OsCl_6 derivative had an Riso of 15.6%, but was only isomorphous to roughly 5Å. It was modeled as 4 sites of occupancy 0.321, 0.207, 0.194 and 0.128, with the highest site at the same position as the second highest

site from K_3IrCl_6.

The initial combination of model and isomorphous replacement phasing did not produce readily interpretable density for gp120. In order to monitor efforts at phase improvement, we devised an objective assay of density quality that used correlations in a region internal to domain 1 of CD4 between the experimental electron density and the calculated model density (CD4 as positioned by molecular replacement and rigid body refinement). Refinement of heavy atom positions improved this correlation, and provided a starting point for phase improvement, primarily using real-space modification techniques (Table 1). These techniques included automatic concatenation of the unmodeled density (with the program PRISM; D. Agard), reciprocal-space averaging of the PRISM modeled density and real-space model subtraction (implemented using the XPLOR(46) shell language), application of real-space constraints such as solvent flattening, histogram matching and negative density truncation (with the program DM (in the CCP4 suite of crystallographic programs), and real-space combinatorial addition of the various experimental density maps (with the program MAPMAN; T.A. Jones). The combinatorial use of these techniques generated greatly improved electron density maps.

At this point, most of the carbon alpha backbone could be modeled (with the program O[47]) defining the secondary structure. Computer aided sequence alignment (slider routine in O) and secondary structure prediction (PHD37) helped to position the amino acid sequence leaving only regions around the N-terminus (residues 79-100 and residues 215-245), the V1/V2 loop, and the V4 loop uncertain. Iterative rounds of building with O, simulated annealing and positional refinement with

XPLOR(46), and addition of ordered solvent clarified the trace.

Structure analysis. Deviations of the CD4 structure in the complex from the free state were measured by the procedure of Wu et al.(10). Deviations were taken as significant when the root mean square (rms) residue deviation was greater than the overall value and also more than 0.5ü greater than variation among the free structures. Interatomic contacts were defined as in Zhu et. al.(48). Structural alignments were made by visual comparison of the SCOP databas, and automatic searches were performed with PrISM (A.-S. Yang and B. Honig).

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Table 1. Structure solution

Data Collection:

	Native	K_3IrCl_6	K_2OsCl_6
Resolution limits (Å)	20-2.5	20-2.8	20-3.5
Total observations	113,966	76,739	25,821
Unique Observations	37,724	28,599	11,982
Rsym (%)*†	9.3(24.7)	11.5(20.2)	14.3(18.2)
Data coverage (%)*	86.0(62.8)	90.8(82.9)	72.5(62.5)

Molecular Replacement:

	Fab	CD4	Fab+CD4
Model	1hil	3cd4/1cdh	1hil+ 1cdh
Scattering (%)¶	43	18	61
Rigid-body correlation#	0.249	0.079	0.325

Generation of experimental electron density:

Phasing Procedure	Correlation coefficient ‡
Molecular replacement (MR)	-0.02
Multiple isomorphous replacement (MIR)	0.34
Phase combination:	
MIR + MR	0.60
+ density modification	0.66
+ density modification + substraction	0.69
Density modelling (concatenation):	
MIR + MR	0.65
+ density modification	0.68
+ density modification + subtraction	0.71
Combination map addition:	0.73

Refinement Statistics:

R-factors (10-2.5 Å):			
Data cutoff (σ)	0	2	4
^{R}crystal (^{R}free) (%)	24.9(32.8)	22.2(30.7)	21.2(29.2)
Data completenes (%)	85.8	77.3	66.4

Geometric parameters (rms):	
Bond length (Å)	0.007
Bond angle (°)	1.59°

B-factors:	average	rms $_{bond}$	rms $_{angle}$
mainchain	20.80	1.33	2.31
sidechain	21.93	1.97	3.01
waters	22.31		

* Rsym = $\Sigma|I_{obs}-I_{avg}|/\Sigma I_{avg}$

† Numbers in parentheses represents the statistics for the shell comprising the outer 10% (theoretical) of the data.

¶ The percentage of scattering of the initial search model.

\# Correlation obtained upon rigid-body refinement of the model against 8-4 û data.

‡ Correlation in the D1 region of CD4 between the experimental electron density and the calculated model density (from CD4 as positioned by molecular replacement) using 10-2.8 û data. Correlations in this region (consisting of ~6000û3) were used to generate a quantitative measure of the overall quality of

the ternary complex experimental electron density. For the purposes of these calculations, the model used for phase combination omitted D1. A correlation of 0.6 is roughly the level of an interpretable protein electron density map, while a well refined structure would give a correlation of about 0.9.

Fourth Series of Experiments

Human immunodeficiency virus (HIV-1) establishes persistent infections in humans leading to the acquired immune deficiency syndrome (AIDS). The HIV-1 envelope glycoproteins, gp120 and gp41, are assembled into a trimeric complex that mediates virus entry into target cells (1). HIV-1 entry depends upon the sequential interaction of the gp120 exterior envelope glycoprotein with the receptors on the cell, CD4 and members of the chemokine receptor family (2-4). The gp120 glycoprotein, which can be shed from the envelope complex, elicits both virus-neutralizing and non-neutralizing antibodies during natural infection. Antibodies that lack neutralizing activity are often directed against the gp120 regions occluded on the assembled trimer and exposed only upon shedding (5,6). Neutralizing antibodies, by contrast, must access the functional envelope glycoprotein complex (7) and typically recognize conserved or variable epitopes near the receptor-binding regions (8-11). Here, we describe the spatial organization of conserved neutralization epitopes on gp120, utilizing epitope maps in conjunction with the X-ray crystal structure of a ternary complex that includes a gp120 core, CD4 and a neutralizing antibody (12). A large fraction of the predicted accessible surface of gp120 in the trimer is composed of variable, heavily glycosylated core and loop structures that surround the receptor-binding regions. Understanding the structural basis for the ability of HIV-1 to evade the humoral immune response should assist vaccine design.

In primary sequence, human and simian immunodeficiency virus gp120 glycoproteins consist of five variable regions (V1-V5) interposed among mor e conserved regions (13). Variable regions V1-V4 form exposed loops

anchored at their bases by disulfide bonds (14).

Neutralizing antibodies recognize both variable and conserved gp120 structures. The V2 and V3 loops contain epitopes for strain-restricted neutralizing antibodies (15-17). More broadly neutralizing antibodies recognize discontinuous, conserved epitopes in three regions of the gp120 glycoprotein (Table 1). In HIV-1 infected humans, the most abundant of these are directed against the CD4 binding site (CD4BS) and block gp120-CD4 interaction (8,9). Less common are antibodies against epitopes induced or exposed upon CD4 binding (CD4i) (18). Both CD4i and V3 antibodies disrupt the binding of gp120-CD4 complexes to chemokine receptors (10, 11). A third gp120 neutralization epitope is defined by a unique monoclonal antibody, 2G12, (19) which does not efficiently block receptor binding (11).

In an accompanying article, (12) we report the X-ray crystal structure of an HIV-1 gp120 core in a ternary complex with two-domain soluble CD4 and the Fab fragment of the CD4i antibody, 17b. The gp120 core lacks the V1/V2 and V3 variable loops, as well as N- and C-terminal sequences, which interact with the gp41 glycoprotein, (6) and is enzymatically deglycosylated (12,21). Despite these modifications, the gp120 core binds CD4 and antibodies against CD4BS and CD4i epitopes (21, 22) and thus retains structural integrity. The gp120 core is composed of an inner domain, an outer domain and a third element, the "bridging sheet" (12) (Figure 34a). All three structural elements contribute, either directly or indirectly, to CD4 and chemokine receptor binding (12). Here, the organization of the surface of the gp120 is analyzed in light of the known antibody responses directed against this exposed viral glycoprotein.

Variability and glycosylation of the gp120 surface

Although generally well-conserved compared with the five variable regions, some variability in the surface of the gp120 core is evident when the sequences of all primate immunodeficiency viruses are analyzed. This variability is disproportionately associated with the surface of the outer domain proximal to the V4 and V5 regions and removed from the receptor-binding regions (Figure 34a,b,c). The L_A, L_C, and L_E surface loops (12) contribute to the variability of this surface. The potential N-linked glycosylation sites present in the gp120 core are concentrated in this variable half of the protein (Figure 34, b and c). In fact, the only conserved residues apparent on this relatively variable surface are asparagine 356 and threonine/serine 358, which constitute a complex carbohydrate addition site within the L_E loop (Figure 34, b and c). Since most carbohydrate moieties may appear as "self" to the immune system, the extensive glycosylation of the outer domain surface may render it less visible to immune surveillance. This helps to explain why antibodies directed against this gp120 surface have been identified so infrequently.

The receptor-binding regions retained in the gp120 core are well-conserved among primate immunodeficiency viruses (12). Also highly conserved is the surface of the inner domain spanned by the α1 helix and located opposite the variable surface described above (Figure 34d). This surface is likely to interact with gp41 and/or with N-terminal gp120 segments absent from the gp120 core. This inner domain surface and the receptor-binding regions are devoid of glycosylation.

Conserved gp120 neutralization epitopes

In conjunction with prior mutagenic and antibody competition analyses (5,6, 18-21), the gp120 core structure reveals for the first time the spatial positioning of the conserved gp120 neutralization epitopes. Although the major variable loops are either absent (V1/V2 and V3) are poorly resolved (V4) in the gp120 core structure, their approximate positions can be deduced (Figure 35a). The conserved gp120 neutralization epitopes are discussed in relation to these variable loops and to the variable, glycosylated core surface.

a) <u>CD4i epitopes</u>. The gp120 epitope recognized by the CD4i antibody, 17b, can be directly visualized in the crystallized ternary complex (12) (Figure 35b,c). Strands from the gp120 fourth conserved (C4) region and the V1/V2 stem contribute to an antiparallel β-sheet (the "bridging sheet" (see Figure 34a)) that contacts the antibody. The vast majority of gp120 residues previously implicated in formation of the CD4i epitopes (18) (Table 1) are located either within this β-sheet or in nearby structures. With the exception of Thr 202 and Met 434, the gp120 residues in contact with the 17b Fab are highly conserved among HIV-1 isolates (Figure 34c, 2a). The prominent ("male") CDR3 loop of the 17b heavy chain dominates the contacts with gp120, with additional contacts through the heavy chain CDR2 (12).

Unusually, there are minimal 17b light chain contacts, leaving a large gap between the gp120 core and most of the 17b light chain surface. In the complete gp120 glycoprotein, this gap is likely occupied by the V3 loop. This is consistent with the position and orientation of the V3 stem on the gp120 core structure

(12), the effect of V3 deletions on the binding of CD4i antibodies in the absence of soluble CD4 (22), the competition of some V3-directed antibodies with CD4i antibodies (5), and the ability of both antibody groups to block chemokine receptor binding (10,11). The chemokine receptor-binding region of gp120 likely consists of elements near or within the "bridging sheet" and the V3 loop (Figure 34a), a model that is supported by recent mutagenic analysis (C. Rizzuto and J. Sodroski, submitted).

The V2 loop likely resides on the side of the 17b epitope opposite the V3 loop (Figure 35a). The V1/V2 loops, which vary from 57 to 86 residues in length (13), are dispensable for HIV-1 replication (22,27), but decrease the sensitivity of viruses to neutralization by antibodies against V3 and CD4i epitopes (27). The latter effect is mediated primarily by the V2 loop (22), suggesting that part of the V2 loop folds back along the V1/V2 stem to mask the "bridging sheet" and adjacent V3 loop. The proximity of the V2 and V3 loops is supported by the observation that, in monkeys infected with simian-human immunodeficiency viruses (SHIVs), neutralizing antibodies are raised against discontinuous epitopes with V2 an V3 components (B. Etemad-Moghadam and J. Sodroski, submitted). The CD4i epitopes are probably masked by the flanking V2 and V3 loops, requiring the evolution of antibodies with protruding ("male") CDRs to access these conserved epitopes. CD4 binding has been suggested to reposition the V1/V2 loops, thus exposing the CD4i epitopes (22). The presence of contacts between the V1/V2 stem and CD4 in the crystal structure (12) is consistent with this model.

b) <u>CD4BS epitopes</u>. CD4 makes a number of contacts within a recessed pocket on the gp120

surface. The gp120-CD4 interface includes two cavities, one water-filled and bounded equally by both proteins, the other extending into the gp120 interior and contacting CD4 only at phenylalanine 43 (Figure 34a (12). Table 1 and Figure 35b,c show the gp120 residues implicated in the formation of CD4BS epitopes recognized by eight representative antibodies. CD4BS epitopes are uniformly disrupted by changes in Asp 368 and Glu 370 (20), which surround the opening of the "Phe 43 cavity." These residues are located on a ridge at the intersection of the two receptor-binding gp120 surfaces, consistent with competition studies suggesting that CD4BS epitopes overlap both the CD4i epitopes and the binding site for CD4 (5,18). The location of the gp120 residues implicated in the formation of the CD4BS epitopes suggests that important elements of the CD4-binding surface of gp120 are accessible to antibodies.

Some CD4BS antibodies, like IgG1b12, are particularly potent at neutralizing HIV-1 (23). IgG1b12 binding is disrupted by gp120 changes that affect the binding of other CD4BS antibodies but, atypically, is sensitive to changes in the V1/V2 stem-loop structure (24). The observation that some well-conserved residues in the gp120 V1/V2 stem contact CD4 (12) raises the possibility that this protruding structure also contributes to the IgG1b12 epitope. This might increase the ability of the antibody to access the assembled envelope glycoprotein trimer, thus increasing neutralizing capability.

While the CD4BS epitopes and the CD4-binding site overlap, several observations demonstrate that the binding of CD4BS antibodies differs from that of CD4.

Changes in Trp 427, a gp120 residue that contacts both the "Phe 43 cavity" and CD4, uniformly disrupt CD4 binding but affect the binding of only some CD4BS antibodies (Table 1). Conversely, some changes in other cavity-lining gp120 residues, Ser 256 and Thr 257, affect the binding of CD4BS antibodies more than the binding of CD4 (20). Since the recessed position of Ser 256 and Thr 257 in the current crystal structure (Figure 35b,c) makes direct contacts with antibody unlikely, either the effects of changes in these residues are indirect or the CD4BS antibodies recognize a gp120 conformation that differs from the CD4-bound state. With respect to the latter possibility, it is interesting that several of the residues implicated in the integrity of the CD4BS epitopes are located in the interface between the inner and outer gp120 domains. CD4BS antibodies might recognize a gp120 conformation in which the spatial relationship between the domains is altered compared with the CD4-bound state, thus allowing better surface exposure of these residues. Differences between the CD4BS epitopes and the CD4-binding site create opportunities for neutralization escape (20). The gp120 residues surrounding the "Phe 43" cavity are highly conserved among primate immunodeficiency viruses (Figure 35a), but the observed modest variation in adjacent surface-accessible residues (e.g., Pro 369, Thr 373 and Lys 432) could account for decrease recognition of the gp120 glycoprotein from some geographic clades of HIV-1 by CD4BS antibodies (24). Additional potential for variation near or within the CD4BS epitopes is created by the unusual water-filled cavity in the gp120-CD4 binding interface, since CD4 binding can apparently tolerate change in the gp120 residues contacting this cavity (12).

The recessed nature of the CD4 binding pocket on gp120 (Figure 34c) may delay the generation of high-affinity

antibodies against the CD4BS epitopes and may afford opportunities to minimize the antiviral efficacy of such antibodies once they are elicited. The degree of recession is probably much greater on the full-length, glycosylated gp120 than is evident on the crystallized gp120 core. The recessed pocket is flanked on one side by the V1/V2 stem-loop structure. The characterization of HIV-1 escape mutants from the IgG1b12 CD4BS antibody and the mapping of several V2 conformational epitopes support a model in which the V2 loop folds back along the V1/V2 stem, with V2 residues 183-188 proximai to Asp 368 and Glu 370. This model is consistent with observations that V1/V2 changes, in combination with V3 changes, can alter the exposure of the adjacent CD4BS epitopes, particularly on the assembled trimer (28). The high temperature factors associated with the V1/V2 stem (12) imply flexibility in this protruding element (Figure 34c,d), expanding the potential range of space occupied by the V1/V2 stem-loop structure. This could enhance masking of the adjacent CD4BS and CD4i gp120 epitopes and divert antibody responses towards the variable loops.

Glycosylation may modify the interaction of antibodies with CD4BS epitopes. The L_D loop, on the rim of the CD4-binding pocket opposite the V1/V2 stem, contains a well-conserved glycosylation site, asparagine 276 (Figure 34c). Changes in this site and at the adjacent alanine 281 have been associated with escape from the neutralizing activity of patient sera (25) and have been seen in SHIVs extensively passaged in monkeys (26). Another conserved glycosylation site at asparagine 386 lies adjacent to both CD4BS and CD4i epitopes (Figure 34c) and could diminish antibody responses against those sites. Additionally, in various HIV-1 strains, carbohydrates are added to the V2 loop segment (residues 186-188) thought to be proximal to the CD4BS epitopes.

c) The 2G12 epitope. The integrity of the 2G12 epitope is disrupted by changes in gp120 glycosylation, either by glycosidase treatment or mutagenic alteration of specific N-linked carbohydrate addition sites (19). These sites are located on the relatively variable surface of the gp120 outer domain, opposite to and approximately 25 A away from the CD4 binding site (Figure 35b,c). The gp120 glycoprotein synthesized in mammalian cells exhibits a dense concentration of high-mannose sugars in this region (Figure 35a). Even in the enzymatically deglycosylated gp120 core, carbohydrate residues constitute much of this surface. 2G12 likely binds at least in part to these carbohydrates, explaining the surprising conservation of the 2G12 epitope despite the variability of the underlying protein surface, which includes the stem of the V3 loop and the V4 variable region. The inclusion of carbohydrate in the epitope might also explain the apparent rarity with which these antibodies are generated. The localization of the 2G12 epitope is consistent with previous studies indicating that 2G12 forms a unique competition group (5,19) and does not interfere with the binding of monomeric gp120 to either CD4 or chemokine receptors (11). Since the 2G12 epitope is predicted to be oriented towards the target cell upon CD4 binding (see below), the antibody may sterically impair interactions of the oligomeric envelope glycoprotein complex with host cell moieties.

Orientation of gp120 in the trimer

Possible orientations of the exterior glycoproteins in the trimer are significantly constrained by the requirement that observed and deduced binding sites for receptors and neutralizing antibodies, sites of N-linked glycosylation, and variable structures be exposed on the surface of he assembled complex. The two-domain CD4 in the ternary complex structure was aligned to the structure of four-domain CD4 (29) to orient the trimer model with respect to the target cell membrane. The consequences of such a model (Figure 36) are:

a) the chemokine receptor-binding sites are clustered at the vertex of the trimer predicted to be closest to the target cell;

b) both variable and conserved neutralization epitopes are concentrated on the half of gp120 facing the target cell;

c) possibilities for intersubunit interactions among the variable structures that could help mask conserved neutralization epitopes are created;

d) the subset of gp120 glycosylation sites to which complex carbohydrates are added in mammalian cells (14) is well-exposed on the outer periphery of the trimer;

e) the highly conserved surface near the α1 helix is available for gp41 and/or gp120 protein interactions within the trimers; and

f) the surface of the assembled envelope glycoprotein complex is roughly hemispherical, thus minimizing the surface area of the viral spike that is potentially exposed to antibodies.

In summary, the X-ray crystal structure of the gp120 core/two-domain CD4/17b Fab complex provides a framework

for visualizing key interactions between HIV-1 and the humoral immune system. Previous antibody competition analyses suggested that the gp120 surface buried in the assembled trimer elicits non-neutralizing antibodies (5,6). By contrast, the binding sites for neutralizing antibodies cluster on a different gp120 surface (5). Our structural studies support the existence of non-neutralizing and neutralizing faces of gp120, and reveal another, immunologically "silent" face of the glycoprotein (Figure 35d). This outer domain surface, along with the major variable loops, contributes to the large fraction of the gp120 surface that is protected against antibody responses by a dense array of carbohydrates and by the capacity for variation. The conserved receptor-binding regions of gp120 represent attractive targets for immune intervention. However, the elicitation of antibodies against these conformation-dependent structures is inefficient. Since the gp120 epitopes near the receptor-binding regions span the inner and outer domains, interdomain conformational shifts may decrease their representation in the immunogen pool. The recessed nature of the CD4-binding site likely contributes to its poor immunogenicity. The sequential recognition of two receptors by primate immunodeficiency viruses allows the conserved elements of the chemokine receptor-binding site to be created or exposed only after CD4 binding has occurred. At that point, it is likely that the proximity of the chemokine-receptor binding site to the cell membrane sterically limits antibody binding. The evolution of primate immunodeficiency viruses that successfully persist despite the host immune response presents challenges to vaccine development. An understanding of the structures of the relevant gp120 epitopes should assist efforts to overcome these hurdles.

Material and Methods

Graphics. Molecular graphics were produced using Midas-Plus (University of California, San Francisco) and GRASP (30).

Assignment of variability. Variability in gp120 residues was assessed using an alignment of sequences derived from approximately 400 HIV-1, HIV-2 and simian immunodeficiency viruses (13). Residues were assigned variability indices and color coded as follows:

- Red : conserved in all primate immunodeficiency viruses;
- Orange: conserved in all HIV-1, including groups M and O and chimpanzee isolates;
- Yellow: some variation among HIV-1 isolates (divergence from the consensus sequence in 1-8 of the 12 HIV-1 groups examined);
- Green : variable among HIV-1 isolates (divergence from the consensus sequence in $\geq$ 9 of the 12 HIV-1 groups examined).

Molecular modeling. Residues 88, 89, and 397-409, which are disordered in the ternary complex crystals (12), were built manually using the program TOM. For the V4 loop (residues 397-409), a dominant constraint was the distance between the ordered residues 396 and 410 ($C\alpha$ - $C\alpha$ distance of 26.88 Å). For the carbohydrate, examination of the N-linked carbohydrate in several crystal structures (e.g. 1fc2, 1gly, 1lte) showed that the core common to both high-mannose and complex N-linked sugars, $(NAG)_2(MAN)_3$ did not differ greatly in conformation after alignment of the first NAG. This core, which represents roughly half the total glycosylation for a typical N-linked site, was built onto each of the 18 consensus N-linked glycosylation sites found on the HXBc2 gp120 core. The

stereochemistry of this initial model was refined using simulated annealing in XPLOR. Briefly, the model was heated to between 2,500° and 3,500°K, and "slow cooled" in steps of 25° to 300°K. At each step, molecular dynamics were performed with the core gp120 fixed, allowing only the modeled residues and carbohydrate (including any attached Asn) to move. The three separate runs, performing molecular dynamics for 5 fs/step, all steric clashes could be removed and the geometry idealized, with an average root mean square (RMS) of carbohydrate movement of only ~3.5Å. Four subsequent runs were made using dynamic times of between 50-75 fs/step. The carbohydrate positions obtained from these runs differed more substantially from those in the starting model (average carbohydrate RMS difference of roughly 8 Å). Two of the models from these longer annealings were much more similar to each other than to the rest (RMS differences in carbohydrate of ~ 4 Å versus ~ 8 Å for all other models). One had been heated to 3,500°K with dynamics of 75 fs/step. The other (shown in the figures display here) was heated to only 2,500°K with dynamics of 50 fs/step. In general the RMS movement of the NAG sugars was roughly half the RMS movement of the MAN sugars, reflecting greater conformational flexibility further from the protein surface.

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Table 1. Conserved Epitopes for Neutralizing Antibodies Identified on the gp120 Core

Competition Group[a]	Examples of Monoclonal Antibodies	gp120 Amino Acids[b]	Probable Mechanism of Virus Neutralization	Characteristics	Selected References
CD4-Binding Site (CD4BS)	F105 15e 21h 1125h 448D 39.3 IgG1b12 830D	Asn 88 (13), Asp 113 (50), Lys 117 (25), Ser 256 (75), Thr 257 (75), Asn 262 (63), Ala 266 (13), Asp 368 (100), Glu 370 (100), Tyr 384 (13), Lys 421 (50), Trp 427 (25), Asp 457 (13), Pro 470 (25), Asp 474 (13), Met 475 (13), Asp 477 (63), Asp/Leu/Tyr 482/483/484 (25)	Interference with gp120-CD4 binding	CD4BS anitbodies compete with CD4 and with antibodies Against CD4i epitopes	8, 9, 20

CD4-Induced Epitopes (CD4i)	17b 48d	Asn 88, Lys 117, Lys 121, Lys 207, Ser 256, Thr 257, Asn 262, ΔV3, Glu 370, Glu 381, Phe 382, Arg 419, Ile 420, Lys 421, Gln 422, Ile 423, Trp 427, Tyr 435, Pro 438, Met 475	Interference with chemokine receptor binding	CD4 binding increases exposure of the epitopes as a result of movement of the V2 variable loop	18 and C. Rizzuto and J. Sodroski, submitted
2G12	2G12	Asn 295, Thr 297, Ser 334, Asn 386, Asn 392, Asn 397	Unknown	Antibody binding is dependent upon proper N-linked glycosylation	19

[a] The gp120 competition groups are defined as Reference 5.

[b] The gp120 amino acids are numbered according to the sequence of the HXBc2 (IIIB) gp120 glycoprotein, where residue 1 is the methionine at the amino-terminus of the signal peptide. Changes in the amino acids listed resulted in significant reduction in antibody binding to the gp120 glycoprotein (Ref. 18-20). The numbers in parentheses indicate the percentage of the CD4BC antibodies examined whose binding is decreased by changes in the indicated residue.

Fifth Series of Experiments

The entry of primate immunodeficiency viruses into target cells depends upon a sequential interaction of the gp120 envelope glycoprotein with the cellular receptors, CD4 and members of the chemokine receptor family. The gp120 third variable (V3) loop has been implicated in chemokine receptor binding, but the use of the CCR5 chemokine receptor by diverse primate immunodeficiency viruses suggests the involvement of an additional, conserved gp120 element. Here we identify a highly conserved gp120 structure that is critical for CCR5 binding, is located adjacent to the V3 loop, and contains neutralization epitopes induced by CD4 binding. This conserved element may be a useful target for pharmacologic or prophylactic intervention in immunodeficiency virus infections.

The clinically abundant primate immunodeficiency viruses behind the β-chemokine receptor CCR5 as an obligate step in virus entry into target cells (1,2). The gp120 glycoproteins of primary, macrophage-tropic HIV-1 strains have been shown to bind specifically to cells expressing CCR5(3,4). The affinity of gp120 binding was increased 2-3 logs by the presence of soluble CD4 (sCD4) (3). Efficient CCR5 binding was dependent upon the presence of the V3 variable loop of gp120, but the gp120 V1/V2 variable loops and N-and C- termini were dispensable for high-affinity binding to CCR5(3). No significant CCR5 binding was observed for gp120 glycoproteins derived from laboratory-adapted HIV-1 isolates, which do not use CCR5 as a coreceptor (3,4).

Specific groups of HIV-1 neutralizing antibodies directed against the gp120 V3 loop or CD4-induced (CD4i) epitopes were able to block the binding of gp120-sCD4 complexes to CCR5-expressing cells (3,4). The CD4i

epitopes are conserved, discontinuous gp120 structures that are exposed better after CD4 binding (5). Mutagenic analysis suggested that elements of the conserved stem of the V1/V2 stem-loop and of the fourth conserved region of gp120 comprise the CD4i epitopes (5). Here we test the hypothesis that conserved gp120 residues near or within the CD4i epitopes are critical for CCR5 binding.

An assay was established that could assess the CCR5-binding ability of a panel of HIV-1 gp120 glycoproteins mutants. The mutants were created by the introduction of single amino acid changes in gp120 residues near or within regions previously shown to be important for the integrity of the CD4i epitopes (5). During the course of this work, structural information on the gp120 epitope recognized by a CD4i-directed antibody, 17b, became available (6) (see below) and was used to guide the mutagenesis. The wtΔ glycoprotein, which lacks the V1/V2 variable loops and the N-terminus and is derived from the YU2 primary macropage-tropic HIV-1 isolate (7), was the starting point for the studies (Fig. 37). This protein was chosen because it had been shown to bind CD4 and CD5 with high affinity (3,8,9). Furthermore, the use of this protein minimized the opportunities for indirect effects of gp120 amino acid changes on CCR5 binding (e.g., by repositioning the V1/V2 loops, which can mask CD4i epitopes (9). Metabolically labeled wtΔ and mutant derivatives were produced in 293T cells and incubated with mouse L1.2 cells stably expressing human CCR5(3), in either the absence or presence of sCD4. The cells were washed and lysed, and bound gp120 protein was detected by precipitation with a mixture of sera from HIV-1 infected individuals (10).

The wtΔ protein efficiently bound to the L1.2 CCR5 cells in the presence of sCD4 (Fig. 38,A and B). Binding was

dramatically reduced when sCD4 was not present in the assay. The wtΔ protein binding to the L1.2-CCR5 cells was inhibited by preincubation of the wtΔ protein with the 17b antibody. Binding was also inhibited by incubation of the L1.2-CCR5 cells with the 2D7 antibody against CCR5 (11) or with the CCR5 ligand, MIP-1β(12). The C11 antibody, which is directed against a gp120 region dispensable for CCR5 binding (3), did not block the binding of the wtΔ protein to the L1.2-CCR5 cells (data not shown). The wtΔ protein did not bind appreciably to the parental L1.2 cells not expressing CCR5, even in the presence of sCD4. These results suggest that the wtΔ protein binds CCR5 in a specific, CD4-dependent manner.

The binding of the panel of gp120 mutants to the L1.2-CCR5 cells in the absence and presence of sCD4 was measured. The recognition of the mutant proteins by sCD4 and by monoclonal antibodies that recognize discontinuous gp120 epitopes (5,13) was assessed in parallel (10). Changes in several gp120 amino acids resulted in dramatic reductions in the ability of the protein to bind to L1.2-CCR5 cells in the presence of sCD4 (Table 1 and Fig. 38C). In some cases (257 T/D, 370 E/Q and 383 F/S), the attenuated CD4-binding ability of the mutant proteins could account for the observed reduction in binding to the L1.2-CCR5 cells. In most cases, however, the mutant proteins that were deficient in CCR5 binding still bound sCD4 and at least one of the monoclonal antibodies recognizing discontinuous gp120 epitopes. As expected, some of the introduced amino acid changes decreased recognition by the 17b antibody. Interestingly, two of the gp120 amino acid changes (437 P/A, 442 Q/L) resulted in an increase in CCR5 binding compared with the wtΔ protein, even though CD4 binding was not significantly increased. In the absence of sCD4, the 437 P/A and 442 Q/L envelope glycoprotein

mutants bound to the L1.2-CCR5 cells slightly better than the other mutants and the wtΔ protein, which exhibited very low levels of binding (Fig. 38A and data not shown).

Recently, the structure of an HIV-1 gp120 core crystallized in a ternary complex with two-domain CD4 and the 17b Fab has been solved (6). The gp120 core is composed of an inner domain, an outer domain, and a "bridging sheet" (Fig. 39A). The "bridging sheet" is a four-stranded, antiparallel β-sheet that includes the V1/V2 stem and strands (β20 and β21) derived from the fourth conserved gp120 region. CD4 contacts gp120 residues in the outer domain and the "bridging sheet" (6). The gp120 residues implicited by our study in CCR5 binding are located near or within the "bridging sheet" (Figure 39, A and B. The "bridging sheet" is predicted to face the target cell after the envelope glycoproteins bind CD4 (6). Even more than the CD4-binding site, the gp120 region implicated in CCR5 binding is highly conserved among primate immunodeficiency viruses; this is particularly apparent in comparison to the remainder of the gp120 surface thought to be exposed on the assembled envelope glycoprotein complex (Fig. 39C) (6). The CD4i epitope for the 17b antibody is located near or within the "bridging sheet" (6), consistent with the ability of the antibody to block CCR5 binding (3,4). All of the individual gp120 residues in which changes disrupted recognition by the 17b antibody (Fig. 39D) are located closed to the gp120-17b interface in the crystallized complex (Table 1). The binding of another antibody, CG10, which disrupts gp120-CCR5 interaction (3) and competes with the 17b antibody for gp120 binding (14), is also affected by changes in amino acid residues within or near the "bridging sheet" (Fig. 39E). The position and orientation of the V3 base in the structure (6), in conjunction with a number of mutagenic and

antibody competition studies (15), suggest that the gp120 V3 loop resides proximal to the region implicated in CCR5 binding (Fig. 39A). For example, the binding of both CG10 and CD4i antibodies to gp120 can be disrupted by some V3 changes (5,14). Furthermore, several V3-directed antibodies compete with CD4i antibdoies for gp120 binding (15).

Our observations suggest that the CCR5-binding site is likely composed of conserved gp120 elements near or within the "bridging sheet" and V3 loop residues. The latter might include more conserved structures (e.g. the aromatic or hydrophobic residue at position 317, altered in this study) as well as more variable structures (16) that determine the specific chemokine receptor used. Some of the gp120 residues identified in this and previous studies (16) as determinants of chemokine receptor utilization could modulate the interaction of the V3 loop and elements near the "bridging sheet". For example, studies of HIV-1 revertants (15) suggested a functional interaction of gp120 residue 440, shown here to influence CCR5 binding, with the V3 loop.

A subset of the gp120 residues in or near the "bridging sheet" likely contacts CCR5 directly. Most of the gp120 residues implicated in CCR5 binding exhibit reasonable solvent accessibility in the free gp120 core (Table 1), consistent with this possibility. The gp120 surface implicated in CCR5 binding is highly basic (6), potentially favoring interactions with the acidic CCR5 amino terminus, which has been shown to be important for gp120 binding (17,18). Additionally, hydrophobic interactions, similar to those seen for gp120-17b binding (6), may also contribute to the gp120-CCR5 interaction.

The exposure and/or formation of the CCR5-binding site

of HIV-1 gp120 glycoproteins is dependent upon interaction with CD4 (3,4). CD4 binding has been shown to reposition the V1/V2 variable loops and thus expose the CD4i epitopes (9), which overlap the CCR5-binding region (3,4). However, since a gp120 glycoprotein lacking the V1 and V2 variable loops also exhibits CD4-dependent CCR5 binding (3), the interaction with CD4 must cause other conformational changes in gp120 related to the CCR5-binding site. Our results, which highlight the proximity of the two receptor-binding sites on gp120, provide likely explanations for the induction of such conformational changes. First, one of the components of the "bridging sheet", the V1/V2 stem, also contacts CD4(6). Thus, CD4 binding, which appears to distort the V1/V2 stem, may reposition this structure and allow the formation of the β-sheet important for CCR5 binding. In this respect, we note that a substitution of aspartic acid for threonine 123, which is located in the V1/V2 stem and contacts CD4, significantly decreases CCR5 binding. This substitution may disrupt CD4-induced conformational changes in the V1/V2 stem required for CCR5 binding. Second, the CD4-bound conformation of gp120 exhibits a cavity (the "Phe 43" cavity) within the gp120 interior(6). This cavity contacts the gp120 inner and outer domains as well as the "bridging sheet" and likely forms as a result of interdomain conformational changes in gp120 induced by CD4 binding(6). Since the "bridging sheet" lacks its own hydrophobic core and is thus dependent upon residues contributed by both inner and outer domains(6), any shift in orientation between these domains would alter the conformation of the "bridging sheet". Furthermore, CD4 binding could also alter the precise orientation of the "bridging sheet" with respect to the inner and outer domains, thus aligning the V3 loop and conserved gp120 elements important for CCR5 binding. To summarize, CD4 binding likely induces conformational changes within the

"bridging sheet" as well as between this sheet and the inner and outer domains to form the high-affinity CCR5 binding site. For some primate immunodeficiency viruses, the CD4-bound conformation of gp120 must be energetically assessable in the absence of CD4 to explain the documented examples of CD4-independent chemokine receptor binding and entry (18,19).

It is likely that the CCR5-binding region defined in this study is also important for the binding of simian and human immunodeficiency viruses to other chemokine receptors. The identified region exhibits one of the most highly conserved surfaces on the HIV-1 gp120 glycoprotein (6), supporting its functional importance for all primate immunodeficiency viruses. The laboratory-adapted HXBc2 envelope glycoprotein, which uses CXCR4 and not CCR5 as a coreceptor (1,2,20), can be converted to an efficient CCR5-using protein simply by substituting the V3 loop of the YU2 virus (2). Thus, all of the CCR5-binding region outside of the V3 loop must be conserved, at least between the HXBc2 and YU2 viruses. Indeed, we have shown that alteration of the lysine 117, lysine 207 and glycine 441 in the HXBc2-YU2V3 chimeric protein also disrupts CCR5 binding (21). Consistent with the use of this region for the binding of other chemokine receptors is the observation (19) that the gp120 changes associated with the conversion of HIV-2 to a CD4-independent, CXCR4-using virus affect the "bridging sheet" and the V3 loop. Alterations in "bridging sheet" residues have also been implicated in changes in the tropism of HIV-1 for immortalized cell lines that do not express CCR5(22). Finally, the 17b antibody neutralizes HIV-1 strains that use different chemokine receptors (5, 14), supporting the involvement fo a common gp120 region in chemokine receptor interaction.

Chemokine receptor binding may trigger additional conformatinal changes in the envelope glycoprotein complex that ultimately lead to the fusion of the viral and target cell membrane. It is believed that some of these changes include exposure of the ectodomain of the gp41 transmembrane envelope gylcoprotein(23). It is interesting that the CCR5-binding region defined herein likely resides closes to the trimer axis of the assembled envelope gycoprotein complex(6). Indeed, some of the gp120 residue changes that affect CR5 binding also affect the non-covalent association of gp120 and gp41 subunits in the trimeric complex(21). These observations raise the possibility that chemokine receptor binding alters the relationship between gp120 and gp41, leading to the exposure of the gp41 ectodomain and interaction with the target cell membrane.

The definition of a highly conserved gp120 structure that this important for binding to CCR5, the major coreceptor used by clinically abundant primate immunologic inhibitors of virus-receptor interactions. An understanding of the CD4-induced conformational changes in this structure may allow the targeting of sucg inhibitors to native or CD4-bound states of gp120.

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10. 293T cells were cotransfected with 20 μg of a plasmid expressing the wtΔ or mutant envelope glycoproteins and 2 μg of a plasmid expressing the HIV-1 Tat protein, using the calcium phosphate technique. Transfected cells were washed and metabolically labeled for 16 hours with 50 μCi/ml ^{35}S-cysteine and 50 μCi/ml(35)S-methionine. Labeled cell supernatants were harvested, cleared by low-speed centrifugation (200 xg for 10 minutes at 4°C) and stored at 4°C until used in the binding assays.

For measurement of the binding of sCD4 and antibodies to the wtΔ and mutant envelope glycoproteins, different dilutions of the envelope glycoprotein-containing supernatants were precipitated to ensure that binding occurred in the linear range of the assay. For CD4 binding, the envelope glycoprotein-containing supernatants were incubated for 30 minutes at room temperature with a concentration of sCD4 (Smith Kline Beecham) empirically determined to precipitate the wtΔ protein optimally. The envelope glycoprotein-sCD4 complexes were then precipitated with the CD4-specific antibody, OKT4 (Ortho) and Protein A-Sepharose (Pharmacia). For binding of the 17b and F105 antibodies, the monoclonal antibodies were preincubated with Protein A-Sepharose prior to overnight incubation with envelope glycoprotein-containing sepernatants at 4°C. For Binding of the CG10 antibody, envelope glycoprotein-containing supernatants were incubated with 100 nM sCD4 at room temperature for 30 minutes prior to addition of a CG10-Protein G-Sepharose mixture and overnight incubation at 4°C. Immunoprecipitates were washed and run on 12.5% SDS-polyacrylamide gels, which were fixed, dried and analyzed by autoradiography. Binding was qualified by densitometry.

To measure CCR5 binding, envelope glycoprotein-containing supernatants were mixed with 100nM xCD4 or phosphate-buffered saline (PBS) and incubated at room temperature for 30-60 minutes. L1.2-CCR5 cells ($2x10^7$cells, LeukoSite, Inc.(3)) were pelleted, resuspended in 500 μl of envelope glycoprotein-containing supernatants, and rocked gently at 37°C for 1 hour. Cells were pelleted, washed twice in PBS and lysed by the addition of NP40 buffer (0.5 M NaCl, 10 mM Tris, pH 7.5, 0.5%

NP40). Lysates were cleared (20,000 xg at 4°C for 15 minutes) in a microdcentrifuge and the envelope glycoproteins were precipitated overnight at 4°C by a mixture of sera from HIV-1-infected individuals and Protein A-Sepharose. Sepharose pellets were washed in NP40 buffer, boiled in SDS-containing sample buffer and run on 12.5% SDS-polyacrylamide gels. Autoradiographed gels were quantitated using a densitometer.

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Table 1. Phenotypes of HIV-1 gp120 mutants. The ability of the wtΔ and mutant glycoptroteins to bind CCR5 expressed on L1.2 cells was determined (10). The recognition of the wtΔ and mutant glycoporteins by sCD4 and monoclonal antibodies was determined (10). All values reported are relatie to those seen for the wtΔ protein. Values represent the average of at least two independent expeiments and exhibitedless than 30% variation from the values shown.

	Ligand Binding‡				
Protein(Fractional Solvent Accessibility)*	CCR5 Binding +	sCD4	17b	CG10	F105
wtΔ	1.00	1.00	1.00	1.00	1.00
107D/R	1.02	1.02	0.97	1.11	1.14
114Q/L	1.22	0.79	0.73	0.71	0.75
117 K/D (0.45)	0.15	0.74	0.64	0.42	0.83
121 K/D (0.57)	0.07	0.73	0.11	0.0	0.99
122 L/S	0.98	0.84	1.07	0.18	1.11
123 T/D (0.49)	0.08	0.99	1.06	0.0	1.25
197 N/D	1.33	1.34	.80	0.81	1.11
199 S/L	1.50	1.32	.94	1.03	1.04
200 V/S	0.84	0.91	1.05	0.49	1.06
201 I/A	0.46	0.90	.67	0.84	0.81
203 Q/L	0.68	0.85	.88	0.52	0.93
207 K/D (0.23)	0.0	0.85	.46	0.13	0.98

209 S/L	1.00	1.11	.85	1.01	1.00
210 F/S	0.65	0.81	.81	0.85	0.74
211 E/K	0.73	1.13	1.03	1.12	1.24
257 T/D	0.05	0.0	.49	0.06	0.0
295 N/E	0.86	0.75	.73	0.98	0.79
308 N/D	0.31	1.10	.89	0.93	1.03
317 L/S	0.08	1.12	1.05	1.13	1.03
330 H/A	0.22	0.75	.55	0.66	0.64
ΔV3 (Δ298-329)	0.0	0.80	0.08	1.27	0.93
370 E/Q	0.17	0.0	1.04	0.12	0.0
372 V/S	0.85	1.03	1.08	1.09	0.44
373 T/D	0.48	1.12	1.10	1.16	1.10
377 N/E (0.04)	0.22	0.71	0.52	0.65	0.60
381 E/R (0.07)	0.07	0.81	0.75	0.29	0.96
383 F/S	0.04	0.0	0.0	0.07	0.0
386 N/D	1.22	1.14	0.97	0.90	0.97
419 R/D (0.82)	0.19	0.86	0.02	0.48	0.82
420 I/R (0.14)	0.06	0.59	0.0	0.72	0.72
421 K/D (0.32)	0.07	0.86	0.19	0.0	0.0
422 Q/L (0.35)	0.07	0.53	0.0	0.20	0.55
423 I/S	0.61	0.97	0.05	0.30	1.03
424 I/S	0.37	0.25	0.48	0.83	0.81
426 M/A	0.75	0.69	0.69	0.72	1.11
429 E/R	1.54	1.17	1.00	1.05	0.82
432 K/A	0.61	1.0	0.92	0.0	1.45
434 M/A	1.22	.90	0.65	0.07	1.04
435 Y/S	0.21	.33	0.22	0.29	1.00
436 A/S	0.98	1.05	0.91	0.99	1.23
437 P/A	1.79	.80	0.68	0.78	0.82
438 P/A (0.28)	0.06	1.18	1.00	1.13	1.18
439 I/A	0.45	0.68	0.76	0.76	0.84
440 R/D (0.43)	0.09	1.03	1.05	1.05	1.13

441 G/V (0.91)	0.0	.67	0.70	0.62	0.78
442 Q/L	2.00	1.11	0.74	1.05	0.83
444 R/D (0.80)	0.25	.79	0.67	0.94	0.74
474 D/R	1.03	.59	0.81	0.74	0.0

*The number of the mutant wtΔglycoproteins is based on the sequence of the prototypic HXBc2 gp120 glycoprotein (24), with 1 representing the initiator methionine. The wild-type YU2 gp120 residue is listed, followed by the subsitituted residue. Amino acid abbreviations: A, Alanine; D, aspartic; E, glutamic acid; F, phenylalanine; G, glycine; h, histidine; I, isoleucine; K, lysone; L, leucine; M, methionine; N, Asparagine; P, proline; Q, glutamine; R, arginine; S, serine; T, threonine; V, valine; Y, tyrosine. The fractional solvent accessibilities associated with gp120 residues in which changes specifically disrupted CCR5 binding are shown in prentheses. Fractional solvent accessibility was claculated as the ratio of solvent-accessible surface area for atoms of amino-acid residue X in the gp120 core (without carbohydrate moieties) to the area obtained after reducing the structure to a Gl-X-Gly tripeptide (24), values cited are for side-chain atoms except for glycine 441 where the value for all atoms is given.

+The binding of the wtΔ glycoprotein to L1.2-CCR5 cells was shown to be linearly related to the concentration of wtΔ protein in the transfected 293T cell supernatants, over the range of concentrations used in these experiments. The total amount of wtΔ and mutant glycoprotein present in the 293T cell supernatants was estimated by precipitation with an excess of a mixture of sera from HIV-1-infected individuals. The amount of wtΔ and mutant glycoprotein bound to the L1.2-CCR5 cells was determined as described (10). The value for CCR5 binding was calculated using the following formula:

$$\text{CCR binding} = \frac{\text{Bound mutant protein}}{\text{Bound wt}\Delta\text{ protein}} \times \frac{\text{Total wt}\Delta\text{ protein}}{\text{Total mutant protein}}$$

‡The recognition of the wtΔ and mutant glycoproteins by sCD4 and antibodies was determined by precipitation of radiolabeled envelope glycoproteins in transfected 293T cell supernatants as described (10). In parallel, the labeled envelope glycoproteins were precipitated with an excess of a mixture of sera from HIV-1-infected individuals. The value for ligand binding was calculated using the following formula:

$$\text{Ligand binding} = \frac{\text{Mutant protein}_{\text{ligand}}}{\text{wt}\Delta\text{protein}_{\text{ligand}}} \times \frac{\text{wt}\Delta\text{protein}_{\text{serum mixture}}}{\text{Mutant protein}_{\text{serum mixture}}}$$

In the sCD4 and 17b columns, the values in bold indicate gp120 residues that exhibit decreased solvent accessibility on the presence of the two-domain sCD4 or 17b Fab, respectively, in the ternary complex (6). Changes in solvent accessibility were calculated using the MS program of Michael Connolly.

What is claimed is:

1. A crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120.

2. The crystal of claim 1, which effectively diffracts X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 4 angstroms or better than 4 angstroms.

3. The crystal of claim 1, which effectively diffracts X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 2.5 angstroms or better than 2.5 angstroms.

4. The crystal of claim 1, wherein the portion of gp120 comprises a CD4 binding site.

5. The crystal of claim 4, further comprising a compound bound to the CD4 site.

6. The crystal of claim 1, wherein the portion of gp120 comprises a chemokine receptor binding site.

7. The crystal of claim 6, further comprising a compound bound to the chemokine receptor binding site.

8. The crystal of claim 1, wherein the portion of gp120 comprises a CD4 binding site and a chemokine receptor binding site.

9. The crystal of claim 8, further comprising of a first compound bound to the CD4 binding site of the polypeptide and a second compound bound to the chemokine receptor binding site of the polypeptide.

10. The crystal of claim 9, wherein the first compound is the second compound.

11. The crystal of claim 9, wherein the crystal is arranged in a space group $P222_1$, so as to form a unit cell of dimensions a=71.6 Å, b= 88.1 Å, c=196.7 Å, and which effectively diffracts x-rays for determination of the atomic coordinates of the gp120 to a resolution of 2.5 Å or better.

12. The crystal of claim 1, wherein the polypeptide is a variant of gp120 lacking the V1, V2, V3, and C5 regions.

13. The crystal of claim 12, wherein the gp120 variant comprises a portion of the conserved stem of the V1/V2 stem-loop structure.

14. The crystal of claim 13, wherein the gp120 variant comprises a portion of the base of the V3 loop.

15. The crystal of claim 14, wherein the gp120 variant comprises a portion of the C5 region.

16. The crystal of claim 1, wherein the polypeptide is a variant of gp120 with 5% by weight of the carbohydrate residues linked to the gp120 in substantially the same manner as they are linked to gp120 in unmodified gp120.

17. The crystal of claim 1, wherein the polypeptide is a variant of gp120 with 15% by weight of the carbohydrate residues linked to the gp120 polypeptide in substantially the same manner as they are linked to gp120 in unmodified gp120.

18. The crystal of claim 12 or 16, further comprising a Fab, a CD4, a polypeptide having amino acid sequence of a portion of CD4, or a combination thereof, bound to the gp120.

19. The crystal of claim 18, wherein the Fab is produced from an antibody to a discontinuous epitope.

20. The crystal of claim 19, wherein the monoclonal antibody is designated 17b.

21. A method for producing a crystal suitable for X-ray diffraction comprising:
    a. deglycosylating a polypeptide having amino acid sequence of a portion of a gp120 wherein said portion is produced by deleting or replacing part of the gp120 to reduce the surface loop flexibility;
    b. contacting the polypeptide with a ligand so as to form a complex which exhibits restricted conformational mobility; and
    c. obtaining crystal from the complex so formed to produce a crystal suitable for X-ray diffraction.

22. The method of claim 21, wherein the V1, V2, or V3 loop of the gp120 contained in the polypeptide are partially truncated, deleted or replaced.

23. The method of claim 21, wherein the polypeptide lacks the V1, V2, V3 and C5 loop of the gp120.

24. The method of claim 21, wherein the ligand is a Fab, a CD4, or a polypeptide having amino acid sequence of a portion of CD4.

25. The method of claim 21, wherein the resulting polypeptide after the deglycosylation contains at least 5% of the carbohydrate.

26. The crystal produced by the method of claim 21.

27. A method for identifying a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
    a. determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and
    b. determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the gp120.

28. A method for designing a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
    a. determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and
    b. designing a compound to fit the binding site.

29. A method of claim 27 or 28, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

30. A method of claim 27 or 28, wherein the atomic coordinates are set forth in Figure 53.

31. A pharmaceutical composition comprising the compound identified by claim 27 and a pharmaceutically acceptable carrier.

32. The method of claim 27, wherein the compound is not previously known.

33. The compound identified by the method of claim 32.

34. The compound designed by the method of claim 28.

35. A composition comprising the compound of claim 34 and a suitable carrier.

36. A method of inhibiting the interaction of HIV-gp120 with CD4 which comprises administering to a mammal a compound, with the proviso that the compound is not CD4, capable of disrupting two or more of the contacts between gp120 and CD4 as set forth in Figure 54.

37. A method for identifying a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:

a. determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and

b. determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the CD4 binding site of the gp120.

38. A method for designing a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120

comprising:

a. determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and

b. designing a compound to fit the CD4 binding site.

39. A method of claim 37 or 38, wherein the crystal further comprising a CD4, a second polypeptide having amino acid sequence of a portion of CD4, or a compound known to be able to bind to the CD4 site of the gp120, bound to the polypeptide.

40. A method of claim 37 or 38, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

41. A method of claim 37 or 38, wherein the atomic coordinates are set forth in Figure 53.

42. A pharmaceutical composition comprising the compound identified by claim 37 and a pharmaceutically acceptable carrier.

43. The method of claim 37, wherein the compound is not previously known.

44. The compound identified by the method of claim 43.

45. The compound designed by method of claim 38.

46. A composition comprising the compound of claim 44

or 45 and a suitable carrier.

47. A method of inhibiting Human Immunodeficiency Virus infection in a subject comprising administering effective of amount of the composition of claim 46 to the subject.

48. A method for identifying a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
   a. determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide comprising the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and
   b. determining whether a compound would fit into the binding site, a positive fit indicating that the compound is capable of binding to the chemokine receptor binding site of the gp120.

49. A method for designing a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
   a. determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide comprising the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and
   b. designing a compound to fit the chemokine receptor binding site.

50. The method of claim 48 or 49, wherein the crystal further comprises a chemokine receptor, a second polypeptide having amino acid sequence of a portion of chemokine receptor, an antibody or a Fab capable of binding to the chemokine receptor binding site or a compound known to be capable of binding to the chemokine receptor binding site, bound to the polypeptide.

51. The method of claim 48 or 49, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

52. The method of claim 48 or 49, wherein the atomic coordinates are set forth in Figure 53.

53. The pharmaceutical composition comprising the compound identified by the method of claim 48 and a pharmaceutically acceptable carrier.

54. The method of claim 48, wherein the compound is not previously known.

55. The compound identified by the method of claim 54.

56. The compound designed by method of claim 49.

57. A composition comprising the compound of claim 55 or 56 and a suitable carrier.

58. A method of inhibiting Human Immunodeficiency Virus infection in a subject comprising administering effective of amount of the composition of claim 57 to the subject, thereby inhibiting Human Immunodeficiency Virus infection.

59. A method of inhibiting the interaction of HIV-gp120

with chemokine receptor which comprises administering to a mammal a compound capable of disrupting two or more of the contacts between gp120 and chemokine receptor as set forth in figure 55, thereby inhibiting the interaction of HIV-gp120 with chemokine receptor with the proviso that the compound is not a chemokine receptor.

60. The method of claim 59, wherein the compound is nonpeptidyl.

61. A substance mimicking the human immunodeficiency virus envelope glycoprotein gp120-binding region of CD4 wherein the size of a residue or analog thereof, corresponding to the phenylalanine at position 43 in the native CD4, is larger than the size of phenylalanine so as to fill the pocket on gp120 which extends beyond position 43 in the gp120/CD4 complex and increase the affinity for gp120.

62. The substance of claim 61, wherein the substance is a peptidomimetic analog, a synthetic polypeptide, a standard polypeptide, or a polypeptide analog.

63. The substance of claim 61, wherein the size of residue or analog thereof is increased by directly or indirectly linking a hydrophobic compound to the residue or analog thereof.

64. The substance of claim 61, wherein the sidechain of the residue or analog thereof is larger than 7 Å across its longest dimension.

65. The substance of claim 61, wherein the sidechain of the residue or analog is larger than 10 Å across its longest dimension.

66. The substance of claim 61, wherein the sidechain of the residue or analog thereof is larger than 15 Å across its longest dimension.

67. The substance of claim 61, wherein the sidechain of the residue or analog thereof is longer than the phenylalanine sidechain's longest dimension.

68. The substance of claim 61, which enhances hydrophobic interactions to residues that line the pocket.

69. The substance of claim 61, which enhances hydrogen bonding to residues that line the pocket.

70. The substance of claim 61, which enhances electrostatic interactions with residues that line the pocket.

71. The substance of claim 61, which enhances surface fit with residues that line the pocket.

72. The substance of claim 61, wherein the residue or analog thereof contains a localization of charge so as to render the gp120-binding region of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

73. The substance of claim 61, wherein the residue or analog thereof contains at least one additional carbon group.

74. The substance of claim 61, wherein the modification involves replacement of the residue at position 43 with a cysteine and substitution of the sulfhydryl group.

75. The substance of claim 61, wherein the modification involves replacement of the residue at position 43 with a tyrosine and substitution of the tyrosine.

76. The substance of claim 61, wherein the residue or analog thereof is directly or indirectly linked to an adaptor.

77. The substance of claim 76, wherein the adaptor residue or analog thereof is directly or indirectly linked to a hydrophobic compound to form a complex.

78. The substance of claim 77, wherein the formed complex is larger than 7 Å across its longest dimension.

79. The substance of claim 77, wherein the complex is larger than 10 Å across its longest dimension.

80. A pharmaceutical composition capable of inhibiting cell entry by human immunodeficiency virus, comprising
  a. an effective amount of the substance of claim 61; and
  b. a pharmaceutically acceptable carrier.

81. A composition capable of inhibiting cell entry by human immunodeficiency virus, comprising
  a. an effective amount of a substance mimicking the human immunodeficiency virus envelope glycoprotein gp120-binding region of CD4 wherein the size of a residue or analog thereof, corresponding to the phenylalanine at position 43 in the native CD4, is larger than the size of phenylalanine so as to fill the pocket on gp120 which extends beyond position 43 in the gp120/CD4 complex and increase the

affinity for gp120; and

b. a suitable carrier.

82. A pharmaceutical composition for treating or preventing human immunodeficiency virus infection, comprising

a. an effective amount of the substance of claim 61; and

b. a pharmaceutically acceptable carrier.

83. A composition for treating or preventing human immunodeficiency virus infection, comprising

a. an effective amount of the substance of claim 61; and

b. a suitable carrier.

84. A method of inhibiting cell entry by human immunodeficiency virus, comprising contacting the cells with an effective amount of the substance of claim 61 to inhibit cell entry by human immunodeficiency virus.

85. A method of treating or preventing human immunodeficiency virus infection in a subject, comprising administering to the subject an effective amount of the substance of claim 61, thereby treating or preventing human immunodeficiency virus infection.

86. A variant of gp120 which presents a hidden, conserved, neutralization epitope.

87. The variant of 86 wherein position 375 is changed from a Serine to a Trptophan.

88. The variant of claim 87 further comprising one of the following changes: 88N to P, 102E to L, 113D to

R, 117K to W, 257T to A, 266A to E, 386N to Q, 395W to S, 421K to L, 470P to G, 475M to S, 485K to V or a combination thereof.

89. A composition comprising the variant of claim 86, 87 or 88 and a suitable carrier.

90. A vaccine comprising the variant of claim 86, 87 or 88.

91. A method for inducing antibody against HIV in a subject comprising adminstering an effective amount of the variant of claim 86 to the subject.

92. The method of claim 91, wherein the subject is a human.

93. The vaccine of claim 91, further comprising a suitable adjuvant.

94. An antibody against the variant of claim 86, 87 or 88.

95. The antibody of claim 94, wherein the antibody is neutralizing to HIV.

96. The antibody of claim 94, wherein the antibody is a monoclonal antibody.

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Filed on	18 June 1998 (18.06.1998)
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(54) Title: CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120, COMPOUNDS INHIBITING CD4-gp120 INTERACTION, COMPOUNDS INHIBITING CHEMOKINE RECEPTOR-gp120 INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS

(57) Abstract: The subject invention provides a crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120. The subject invention also provides the above-described crystals, wherein the crystal is arranged in a space group $P222_1$, so as to form a unit cell of dimensions a=71.6 Å, b=88.1 Å, c=196.7 Å, and which effectively diffracts X-rays for determination of the atomic coordinates of the gp120 to a resolution of 2.5 Å or better. The subject invention additionally provides compounds inhibiting the CD4-gp 120 interaction, compounds inhibiting chemokine receptor-gp120 interaction, mimics of CD4, gp120 variants and uses thereof.

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FIG. 1

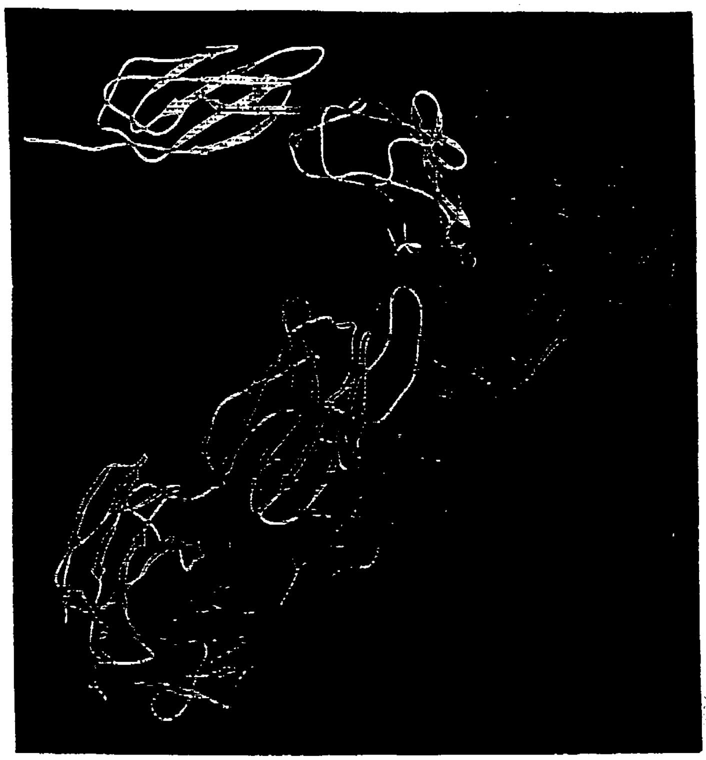


FIG. 2

gp120/17/CD4 Complex Structure

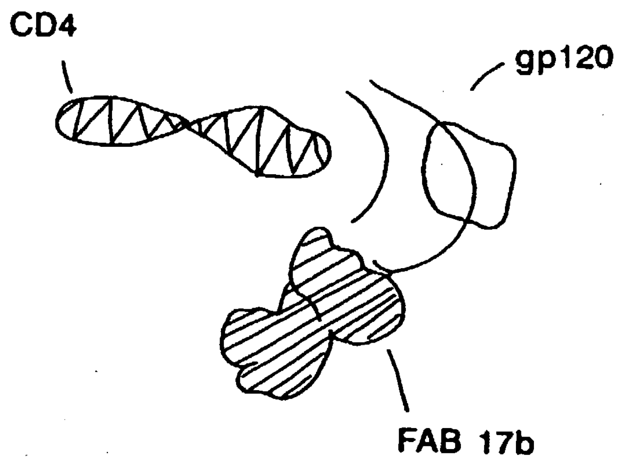


FIG. 3B FIG. 3D FIG. 3F

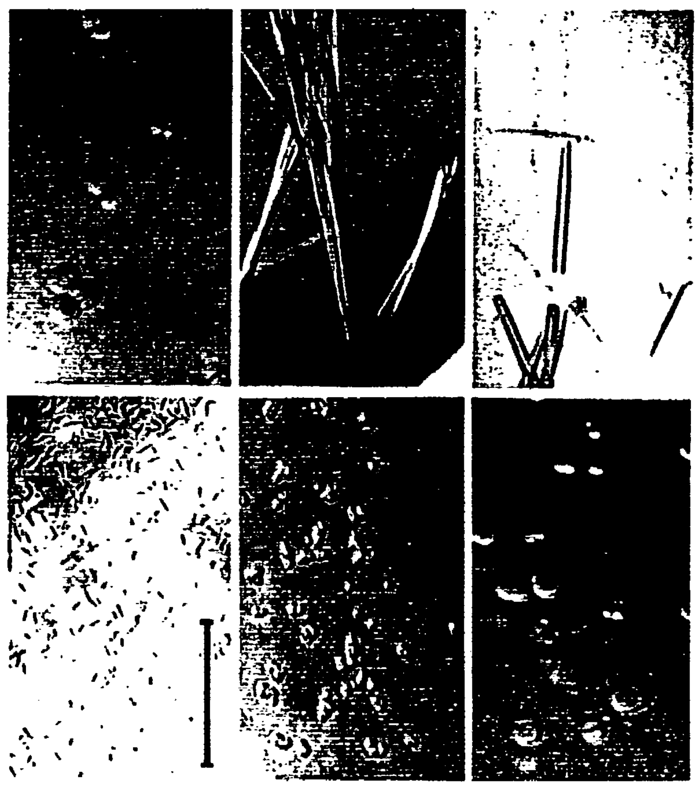


FIG. 3A FIG. 3C FIG. 3E

FIG. 4


1 2 3 4 5
Δ82ΔV1/2*ΔV3ΔC5
Fab 17b
D1D2 sCD4
Δ82ΔV1/2*ΔV3ΔC5
Fab 17b
D1D2 sCD4

FIG. 5A

FIG. 5B

FIG. 6

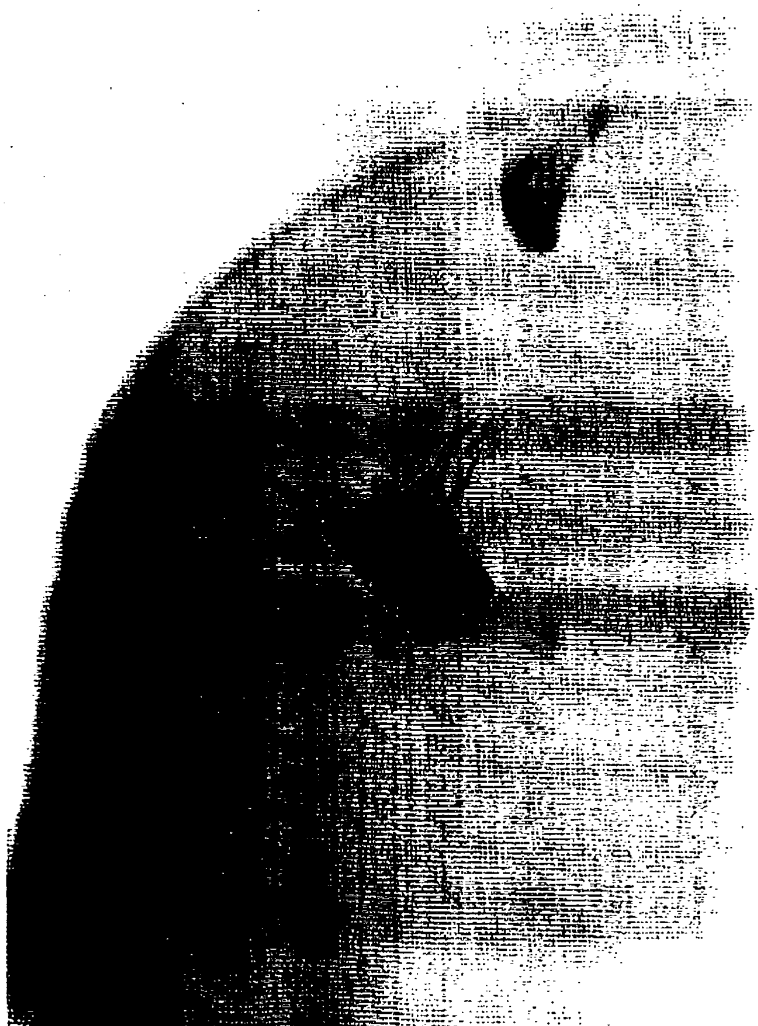


FIG. 7

FIG. 8

FIG. 9

FIG. 10

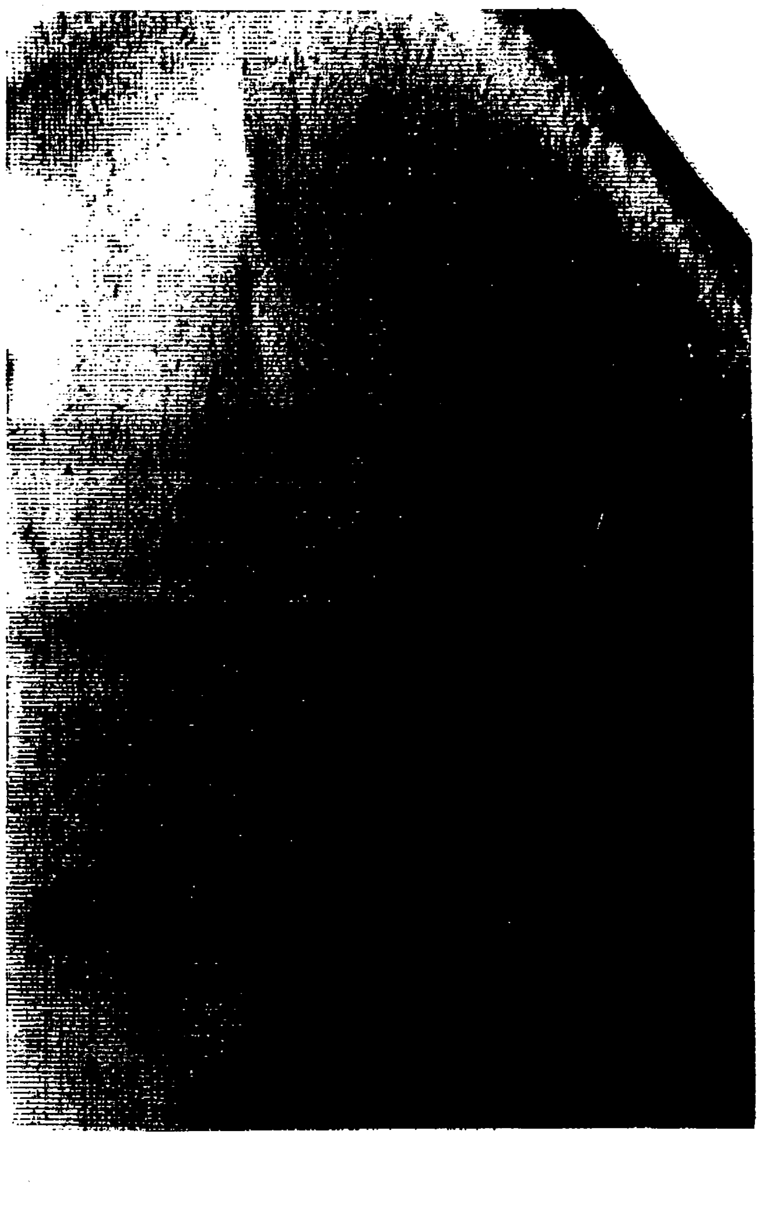


FIG. 11

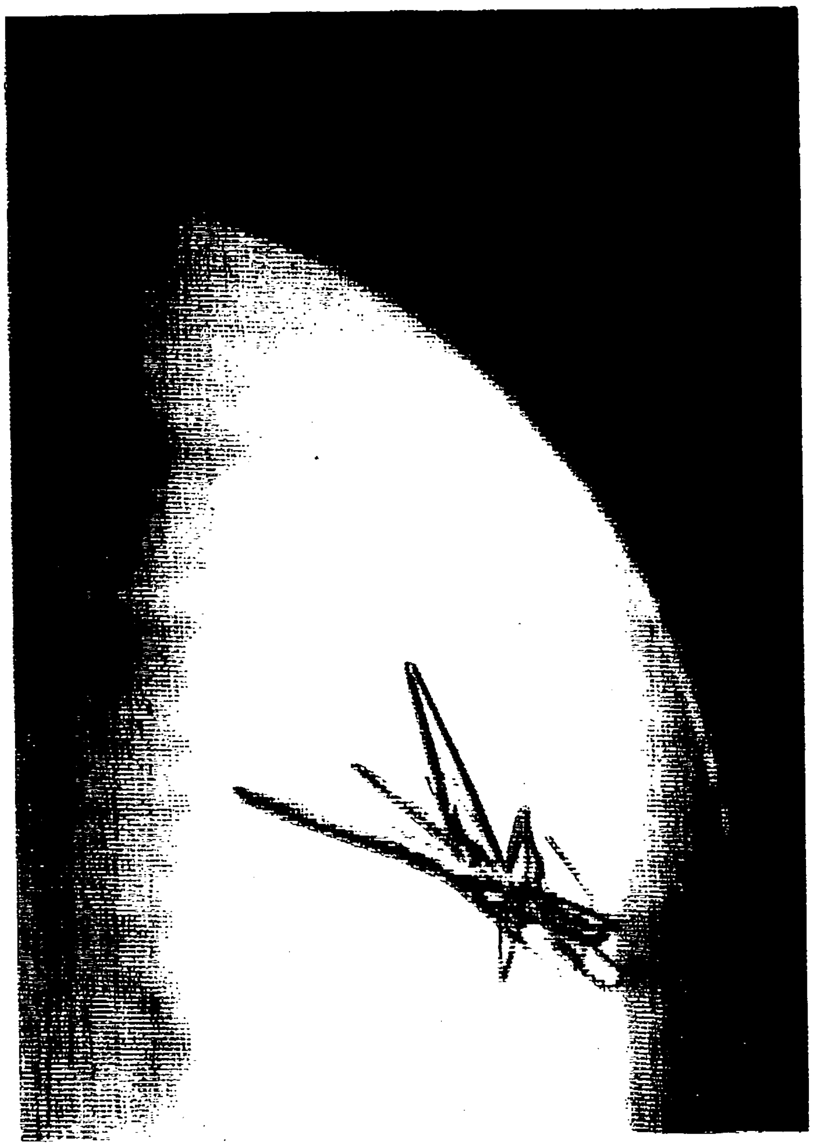


FIG. 12

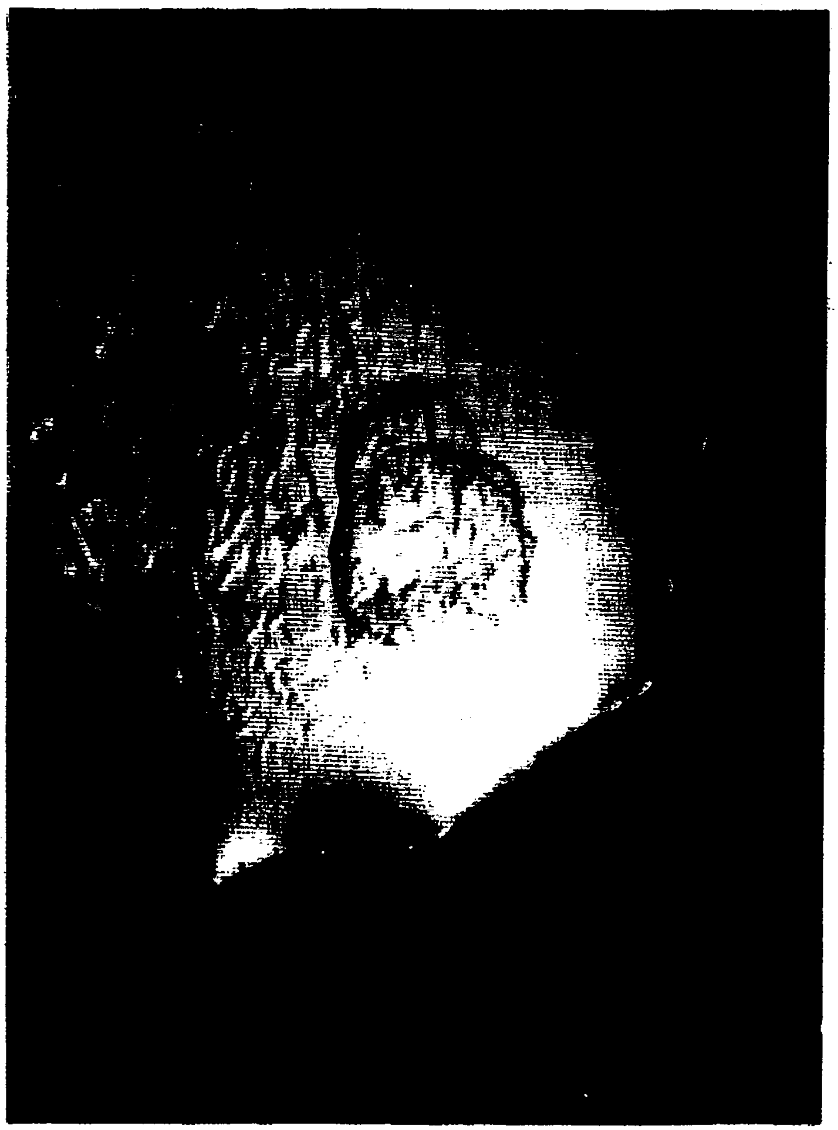


FIG. 13

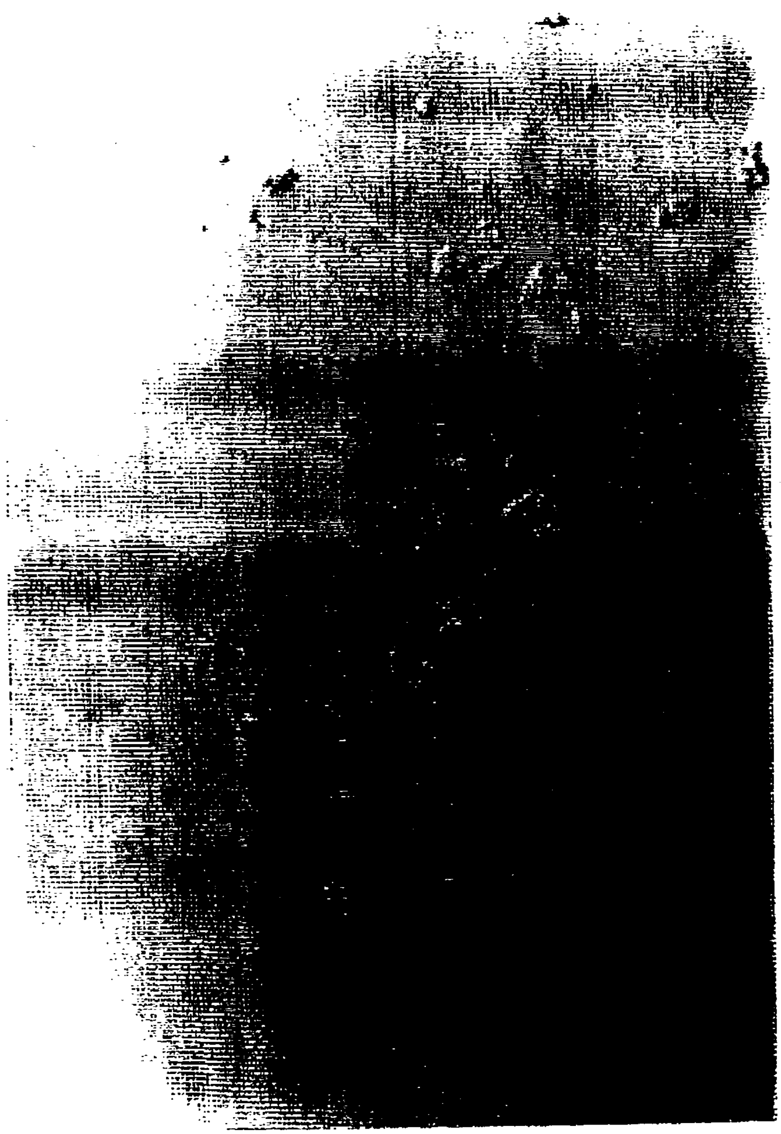


FIG. 14

FIG. 15

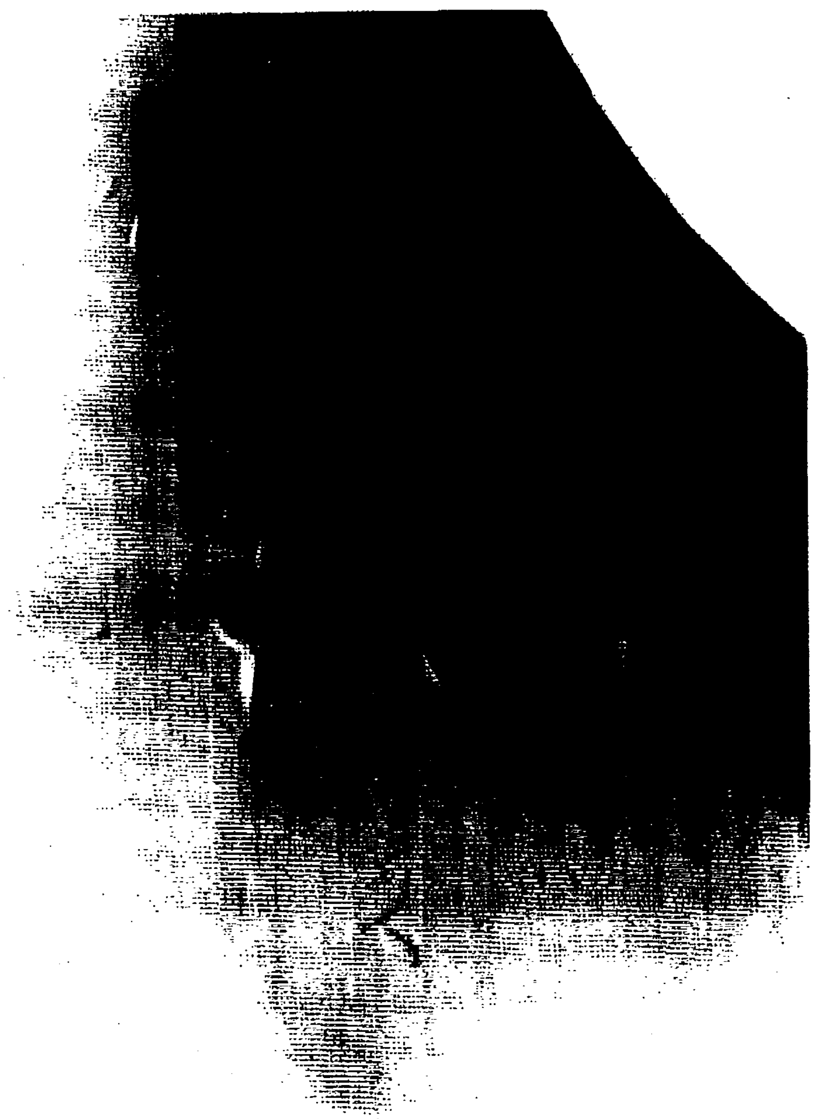


FIG. 16

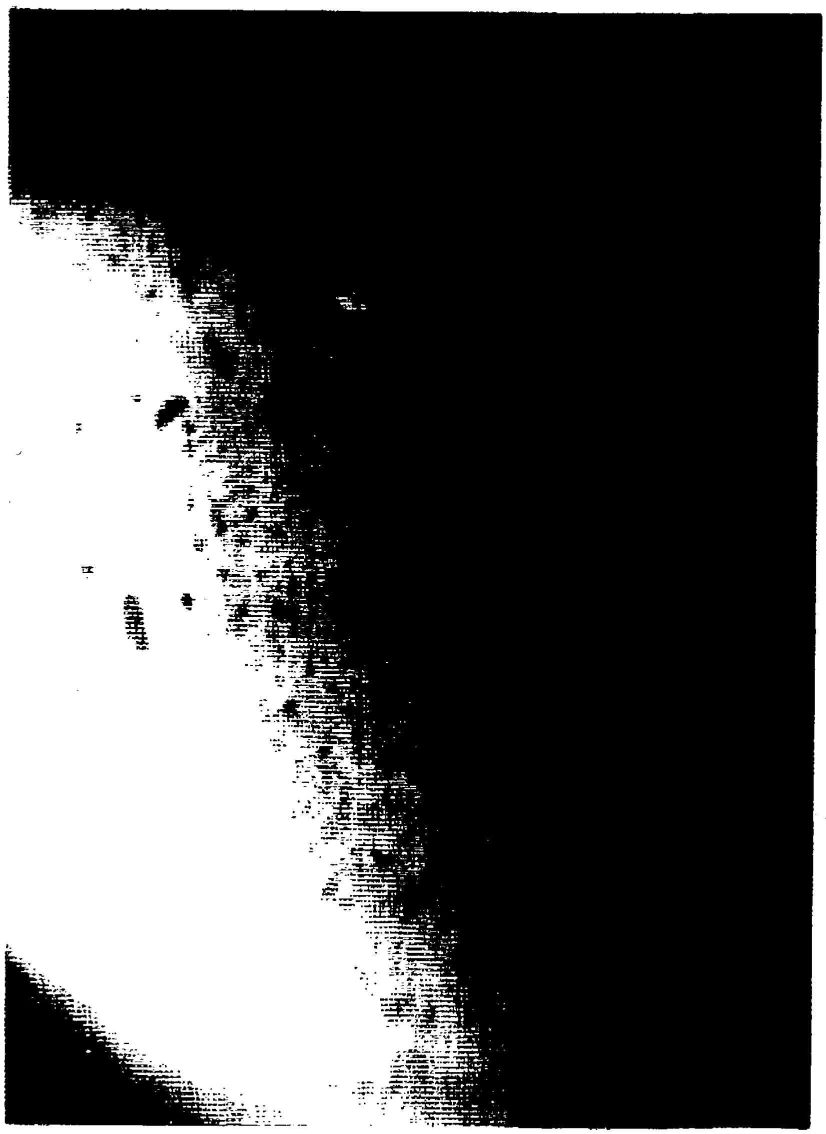


FIG. 17

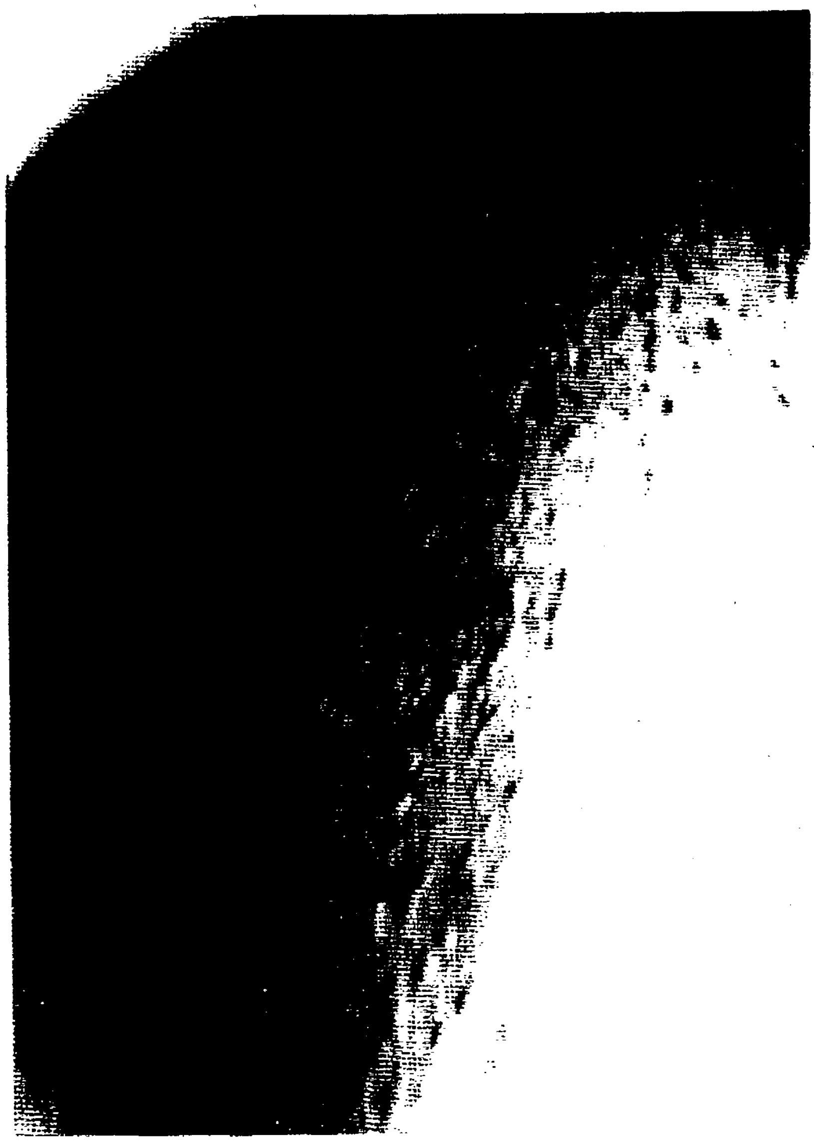


FIG. 18

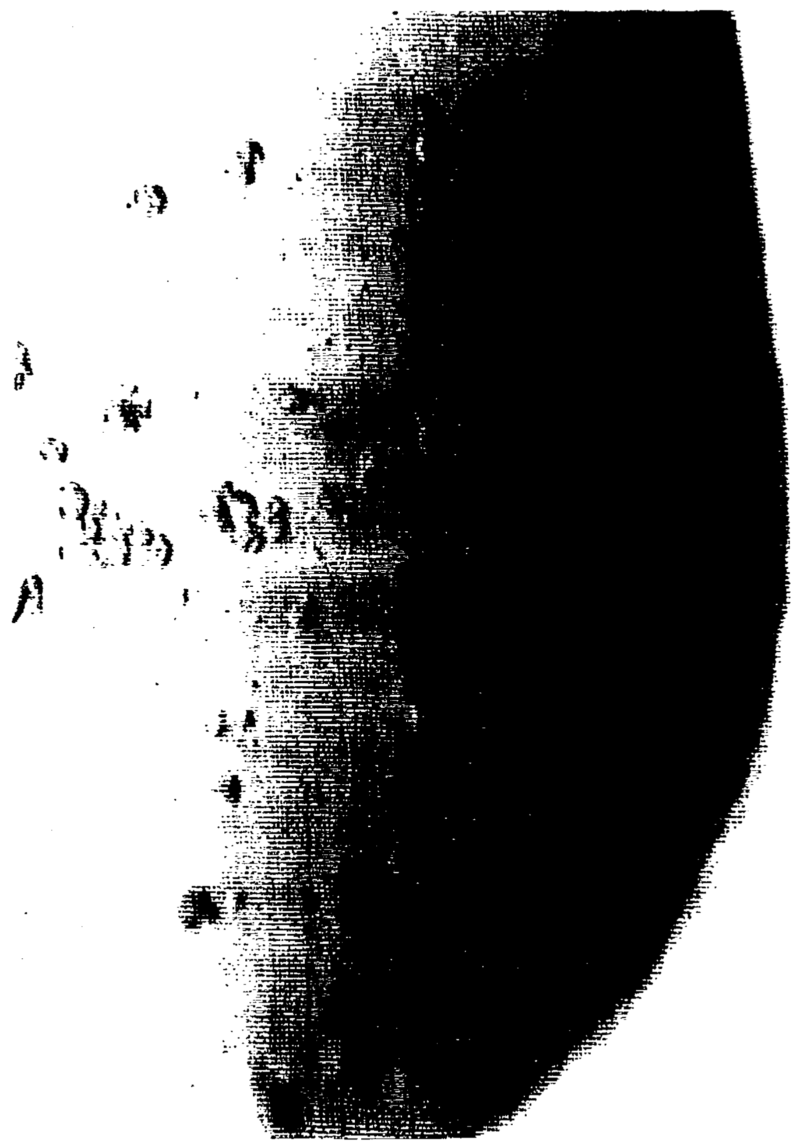


FIG. 19

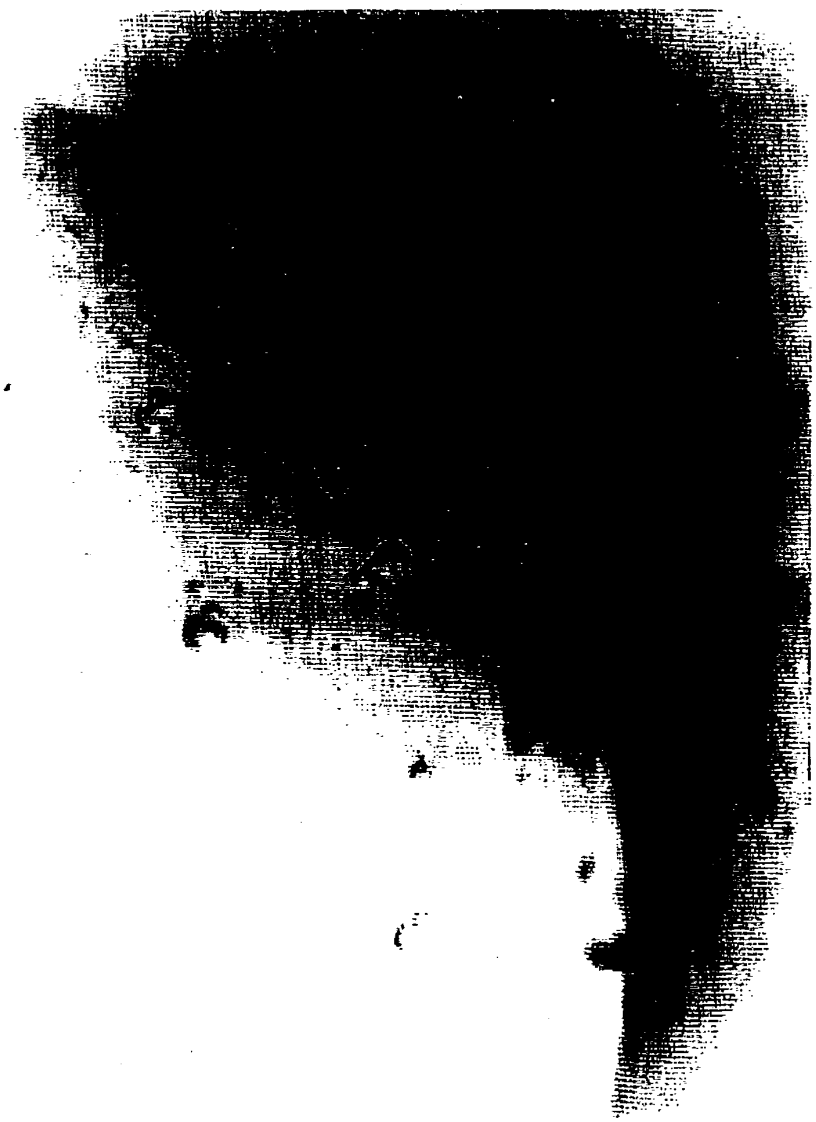


FIG. 20

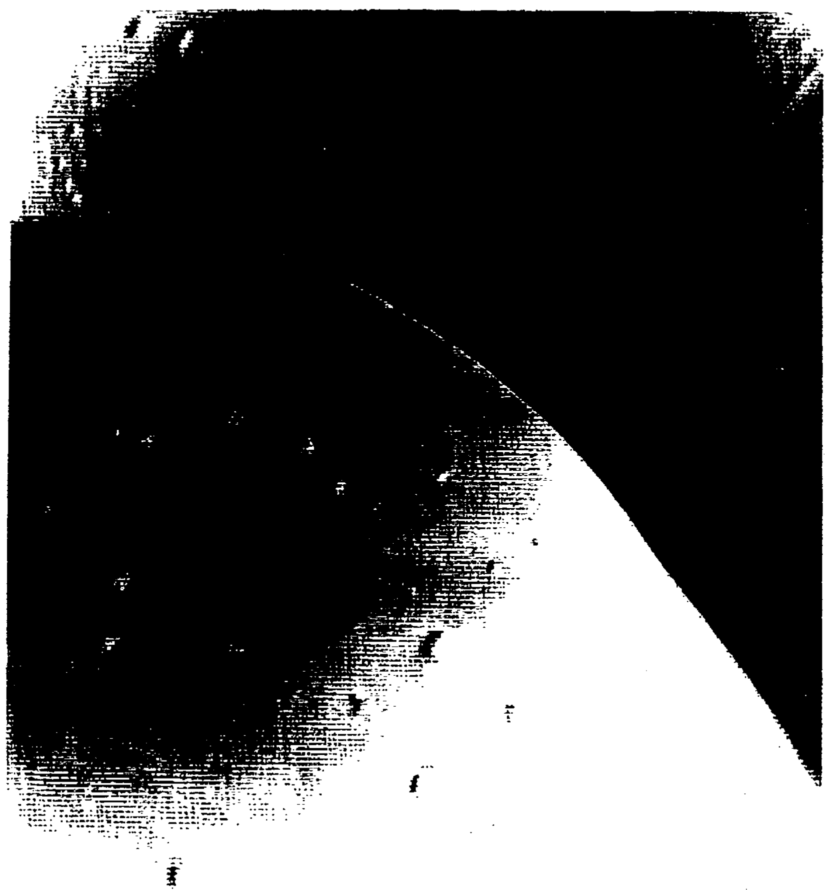


FIG. 21

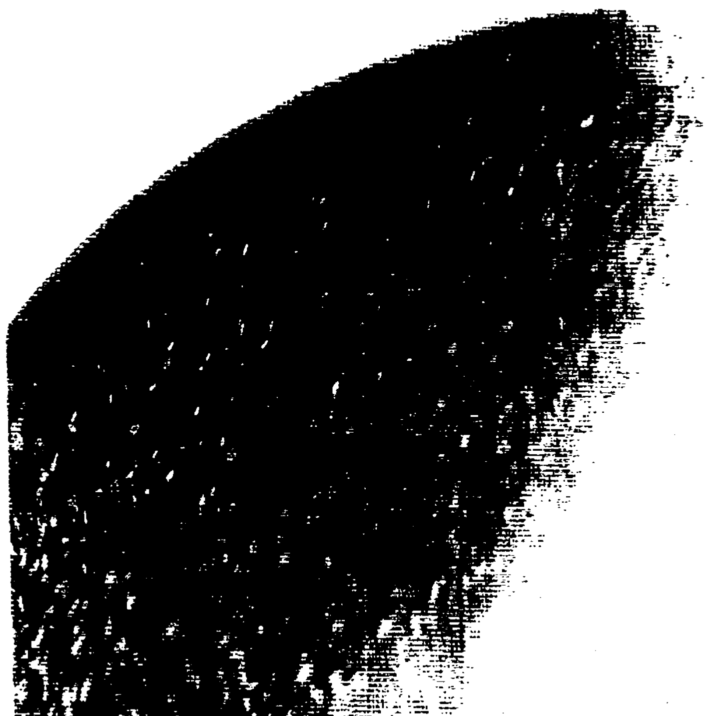


FIG. 22

FIG. 23

FIG. 24

FIG. 25

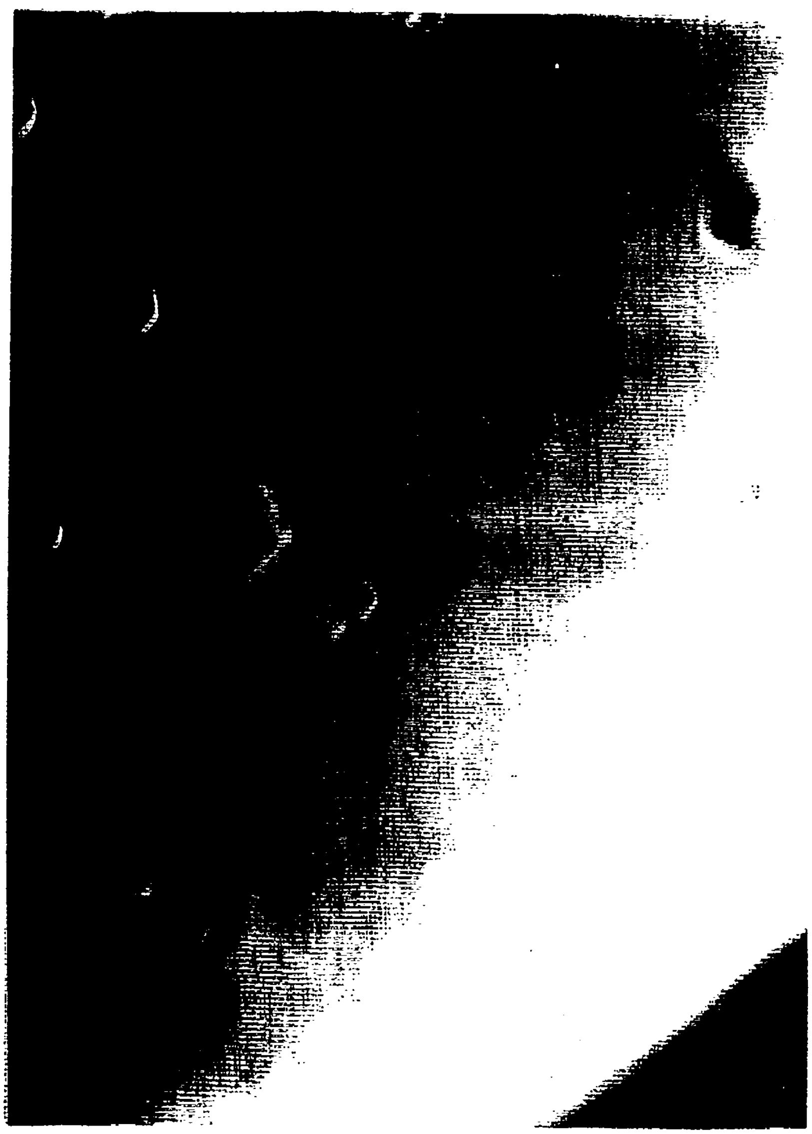


FIG. 26A

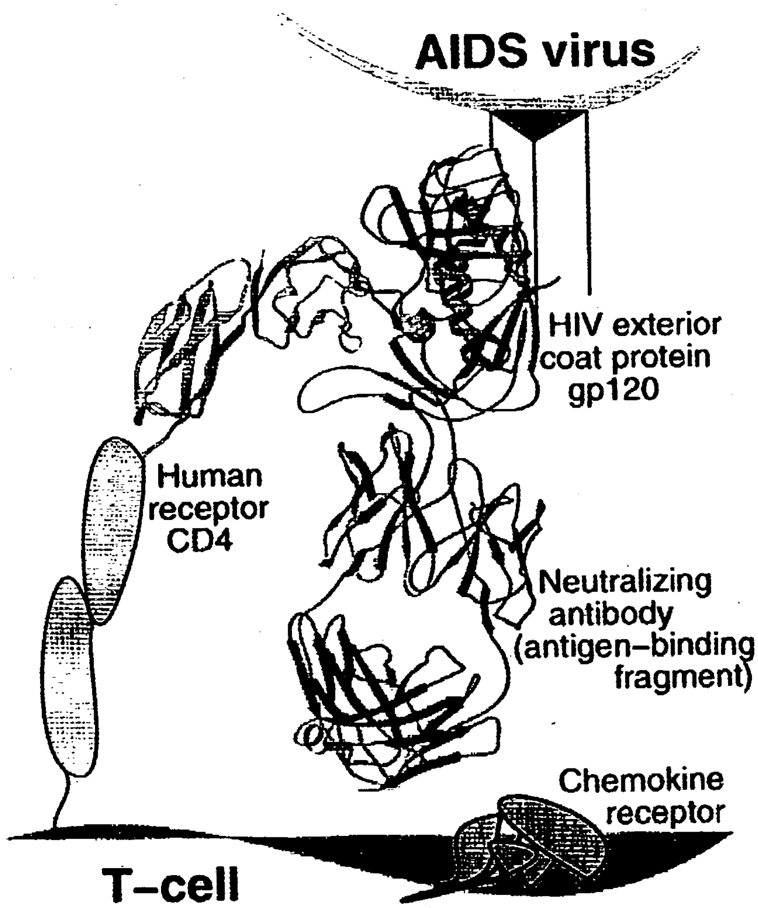

AIDS virus
HIV exterior
coat protein
gp120
Human
receptor
CD4
Neutralizing
antibody
(antigen-binding
fragment)
Chemokine
receptor
T-cell

FIG. 26B

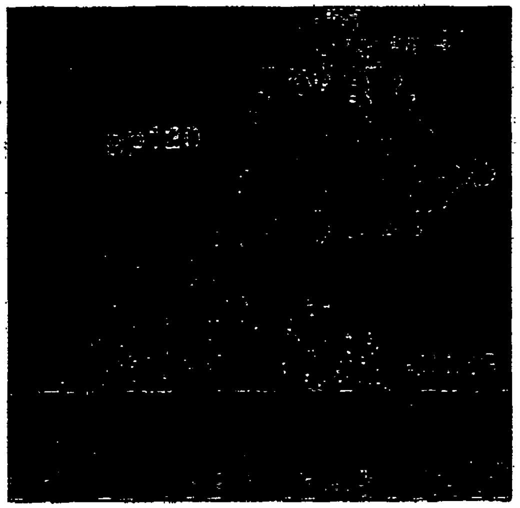


FIG. 27A

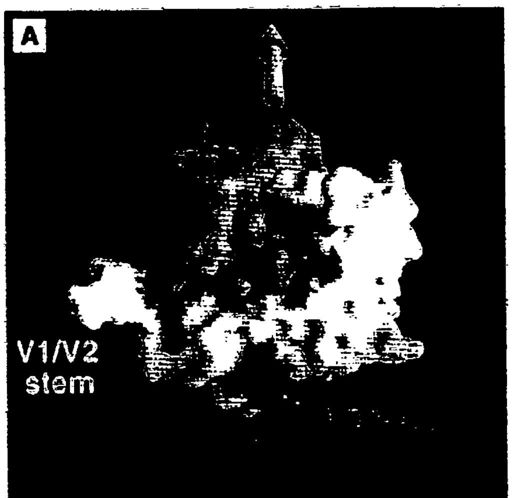
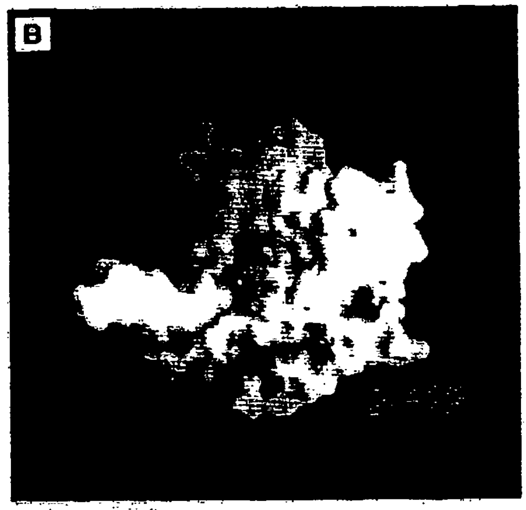


FIG. 27B



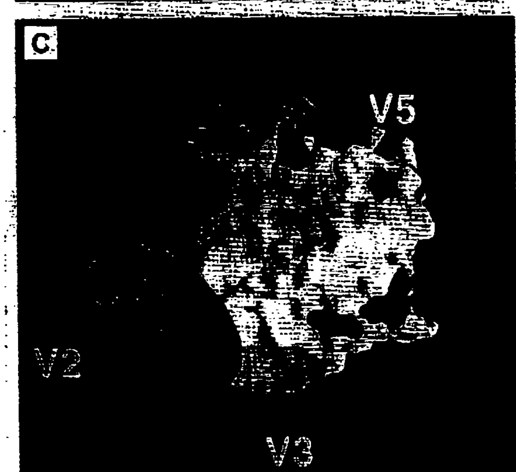


FIG. 27C

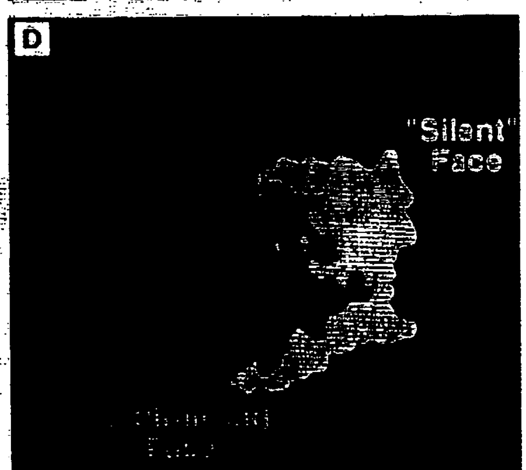


FIG. 27D

FIG. 28

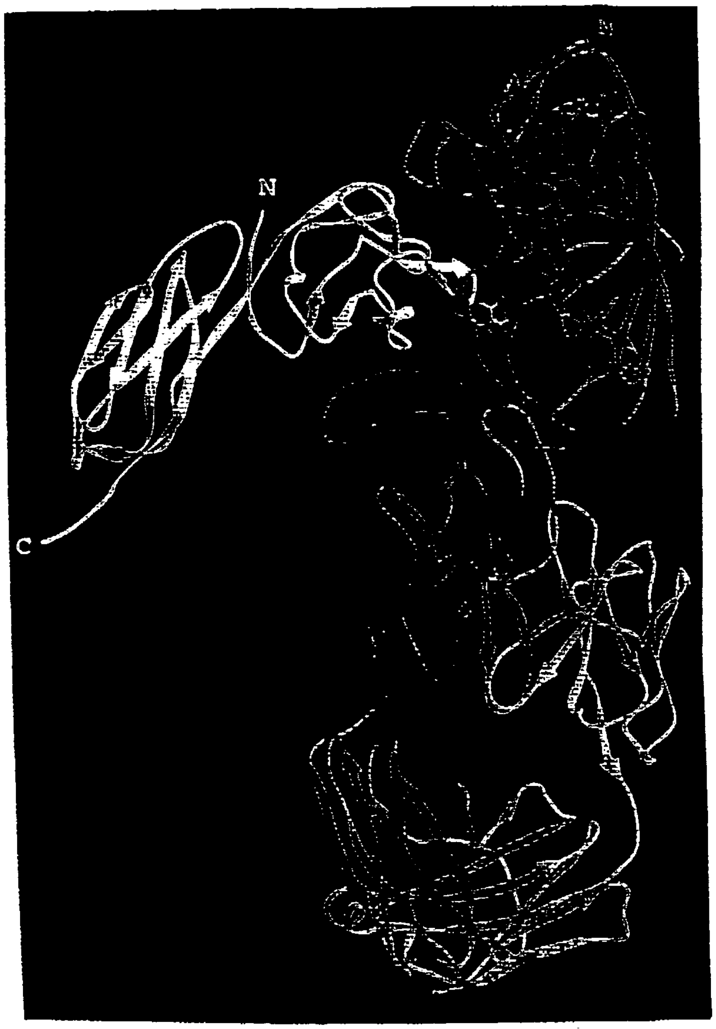
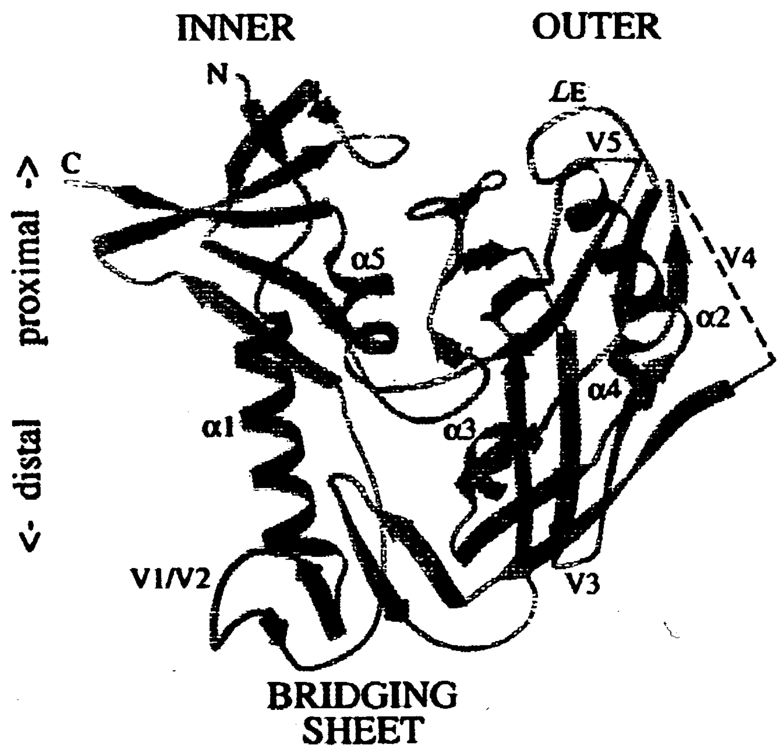


FIG. 29A


INNER
OUTER
N
C
proximal ->
<- distal
α5
α1
V1/V2
LE
V5
V4
α2
α4
α3
V3
BRIDGING
SHEET

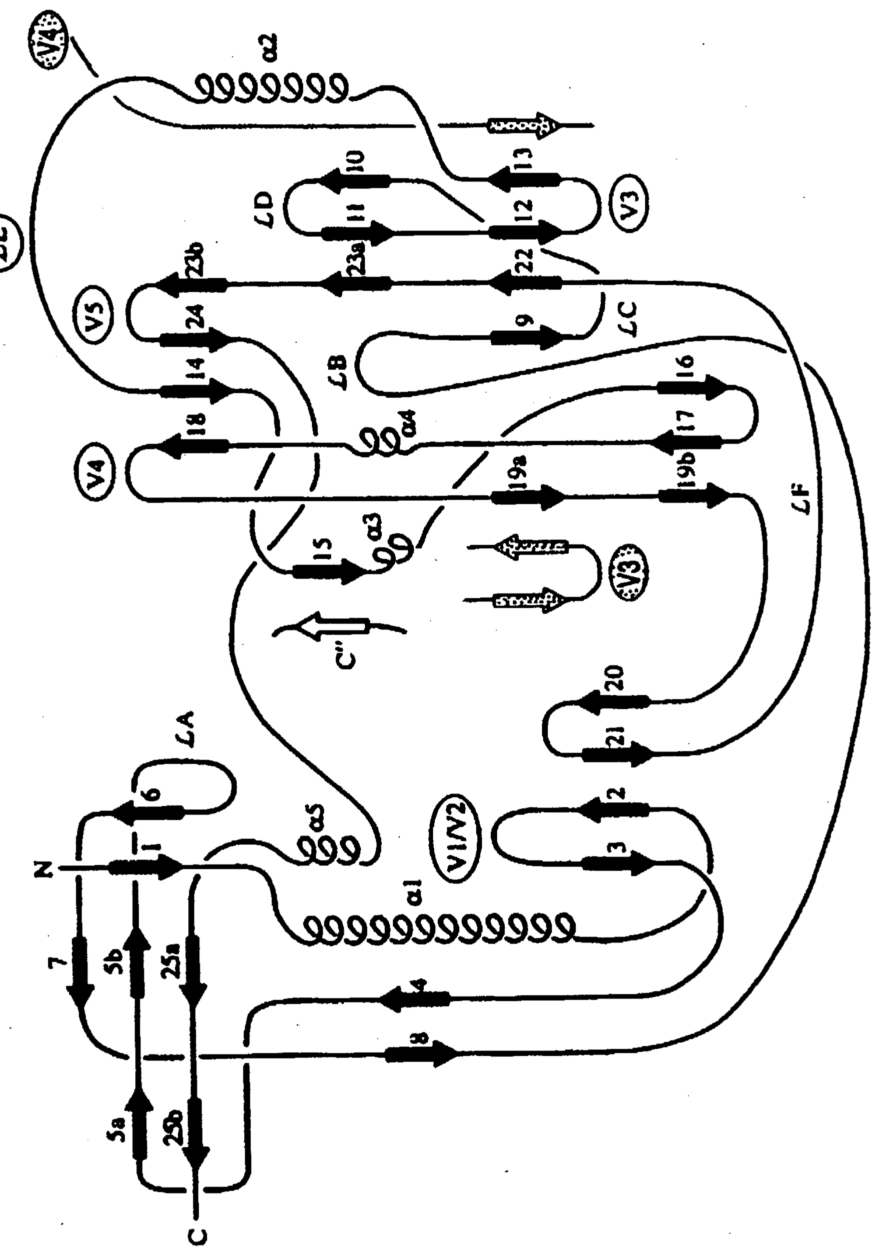


FIG. 29B

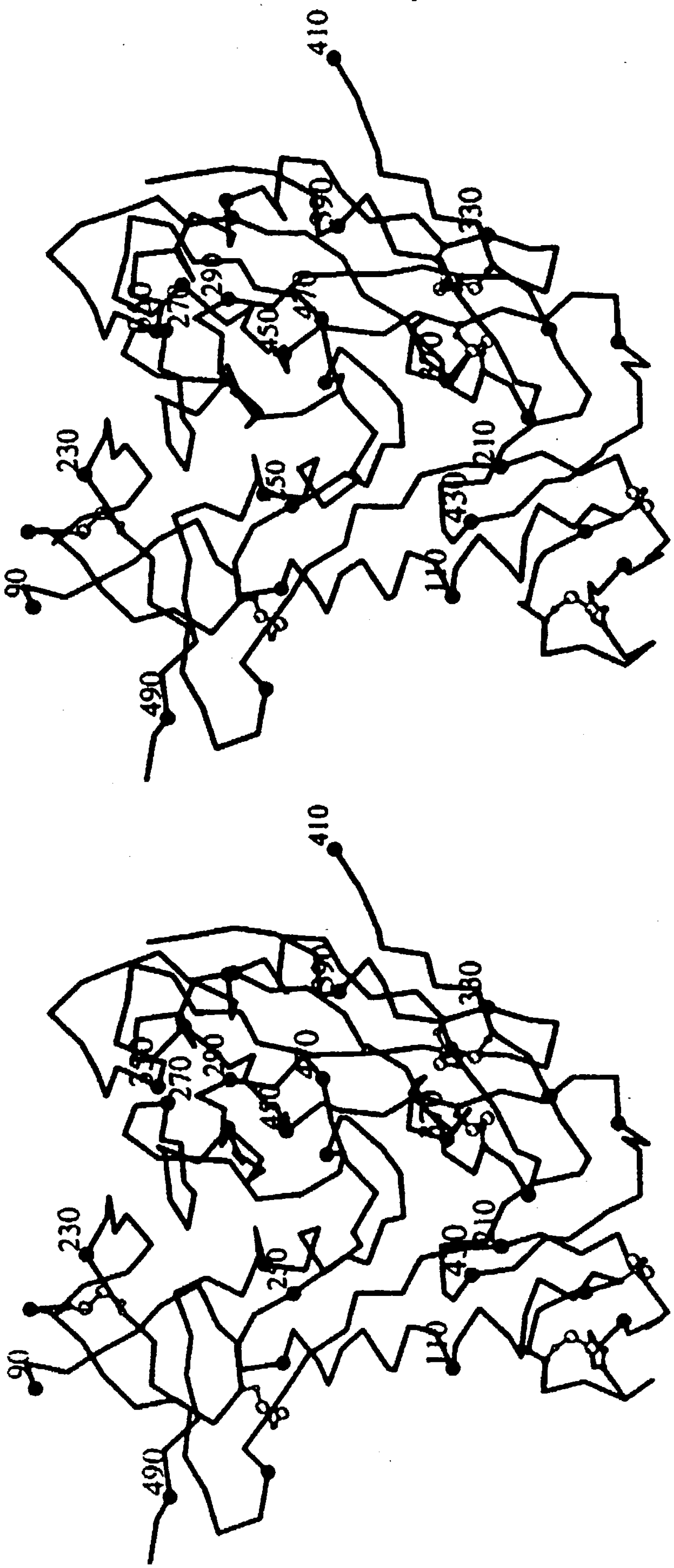


FIG. 29C

FIG. 29D-1

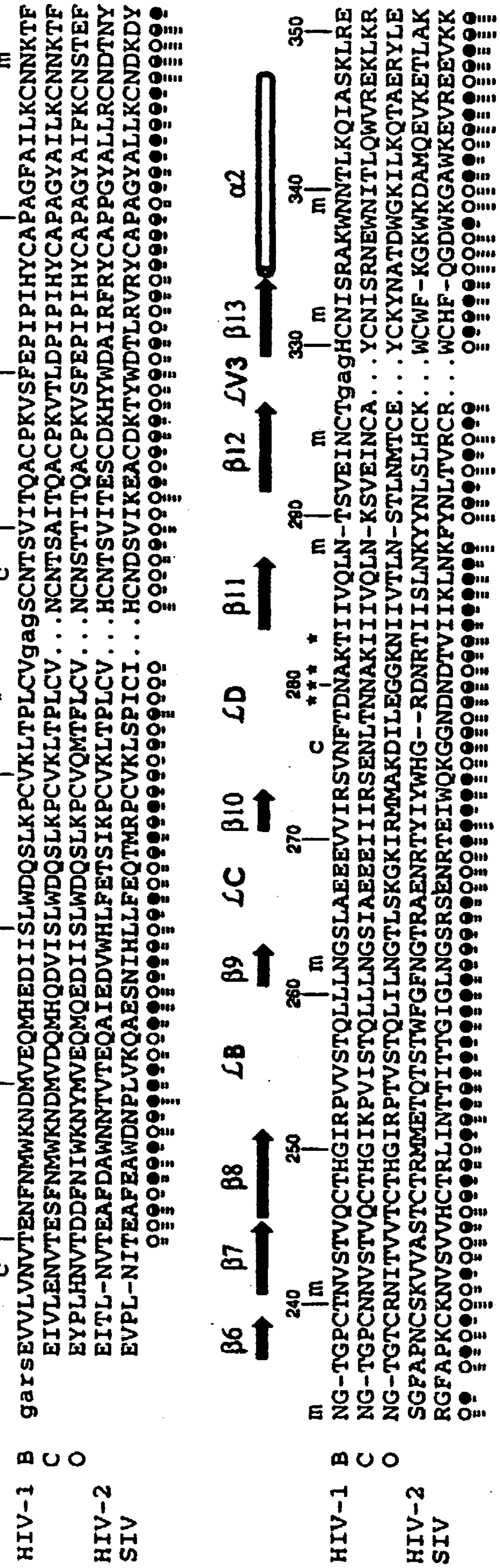


FIG. 29D-2

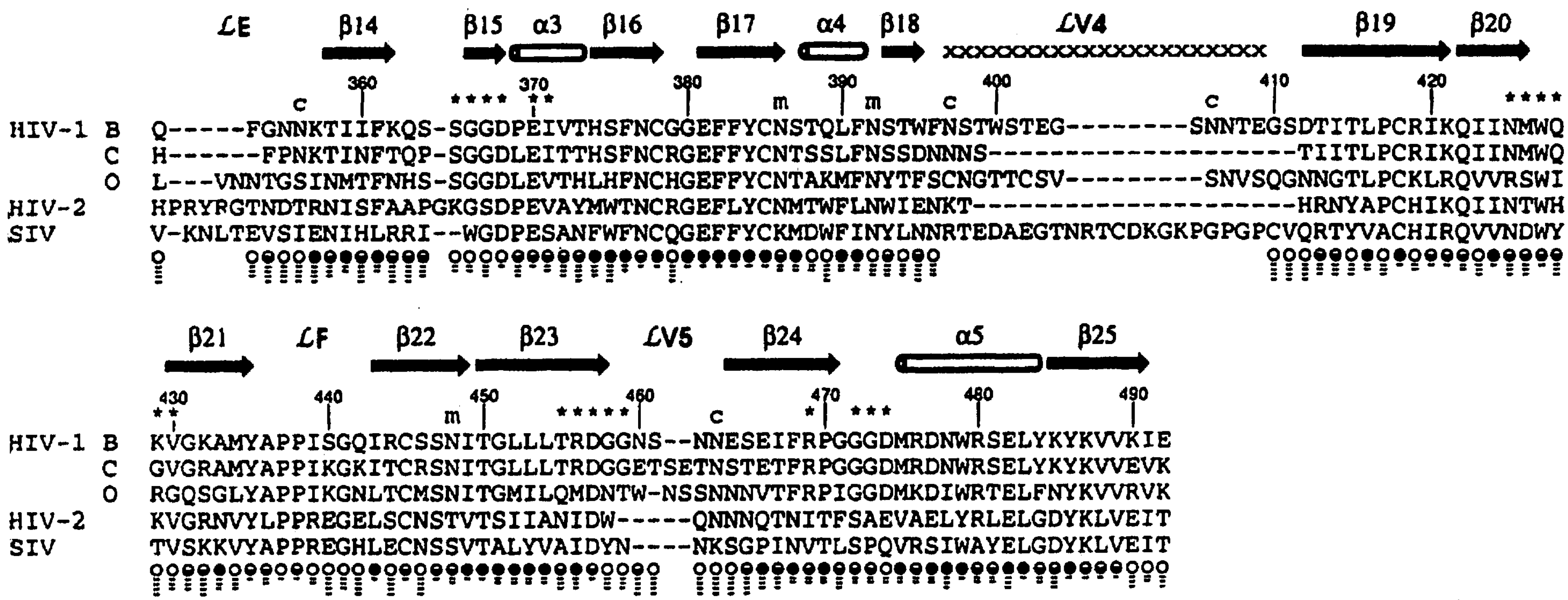

ℒE β14 β15 α3 β16 β17 α4 β18 ℒV4 β19 β20
360 370 380 390 400 410 420
HIV-1 B Q-----FGNNKTIIFKQS-SGGDPEIVTHSFNCGGEFFYCNSTQLFNSTWFNSTWSTEG--------SNNTEGSDTITLPCRIKQIINMWQ
C H------FPNKTINFTQP-SGGDLEITTHSFNCRGEFFYCNTSSLFNSSDNNNS-------------------TIITLPCRIKQIINMWQ
O L---VNNTGSINMTFNHS-SGGDLEVTHLHFNCHGEFFYCNTAKMFNYTFSCNGTTCSV---------SNVSQGNNGTLPCKLRQVVRSWI
HIV-2 HPRYRGTNDTRNISFAAPGKGSDPEVAYMWTNCRGEFLYCNMTWFLNWIENKT--------------------HRNYAPCHIKQIINTWH
SIV V-KNLTEVSIENIHLRRI--WGDPESANFWFNCQGEFFYCKMDWFINYLNNRTEDAEGTNRTCDKGKPGPGPCVQRTYVACHIRQVVNDWY
β21 ℒF β22 β23 ℒV5 β24 α5 β25
430 440 450 460 470 480 490
HIV-1 B KVGKAMYAPPISGQIRCSSNITGLLLTRDGGNS--NNESEIFRPGGGDMRDNWRSELYKYKVVKIE
C GVGRAMYAPPIKGKITCRSNITGLLLTRDGGETSETNSTETFRPGGGDMRDNWRSELYKYKVVEVK
O RGQSGLYAPPIKGNLTCMSNITGMILQMDNTW-NSSNNNVTFRPIGGDMKDIWRTELFNYKVVRVK
HIV-2 KVGRNVYLPPREGELSCNSTVTSIIANIDW-----QNNNQTNITFSAEVAELYRLELGDYKLVEIT
SIV TVSKKVYAPPREGHLECNSSVTALYVAIDYN----NKSGPINVTLSPQVRSIWAYELGDYKLVEIT

FIG. 30A

FIG. 30B

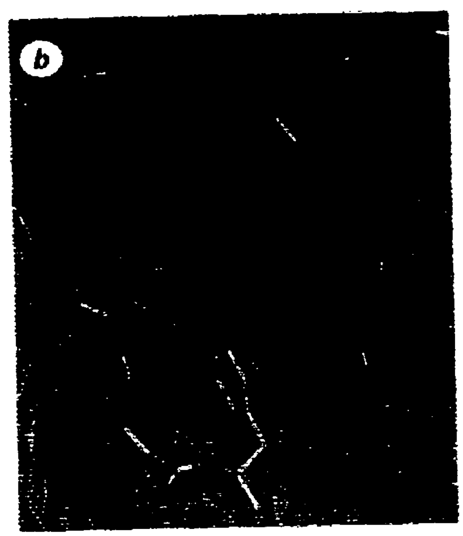


FIG. 30F

FIG. 30G

FIG. 30H

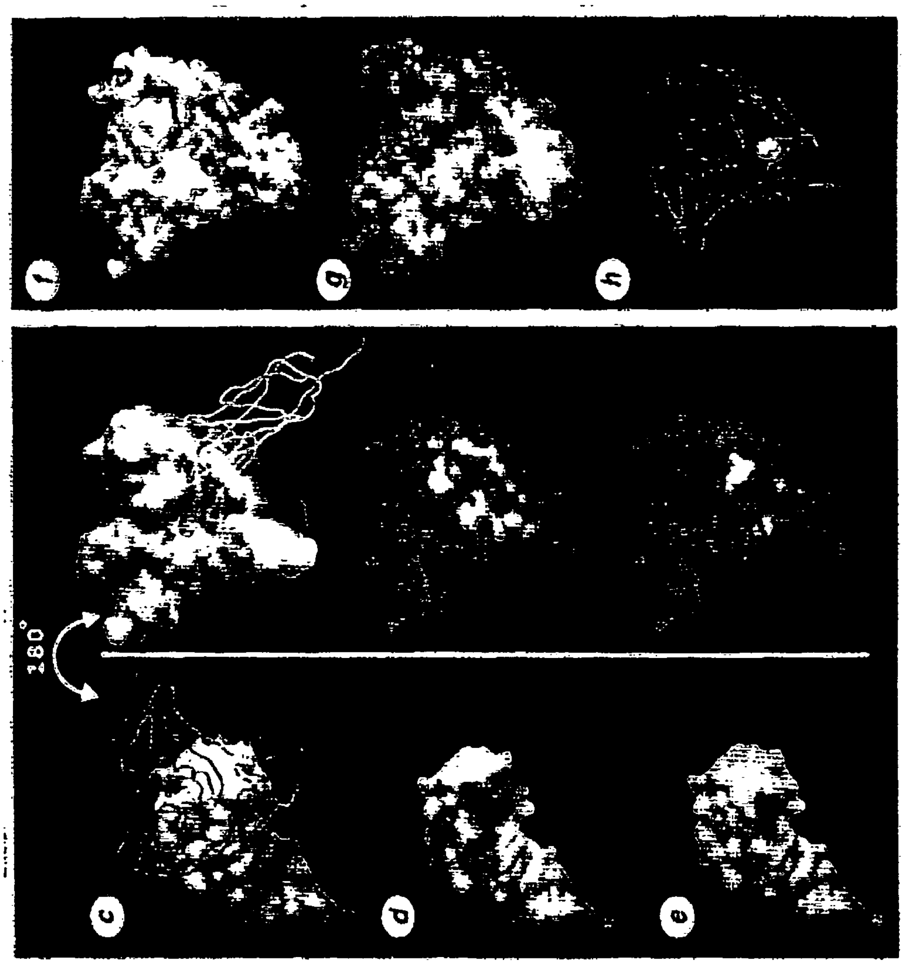


FIG. 30C

FIG. 30D

FIG. 30E

FIG. 30I

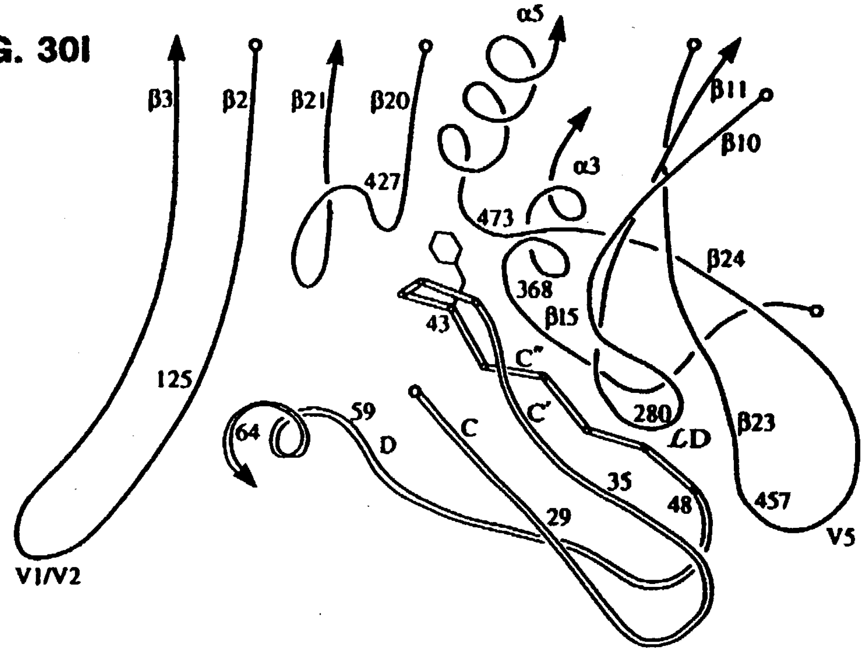


FIG. 30J

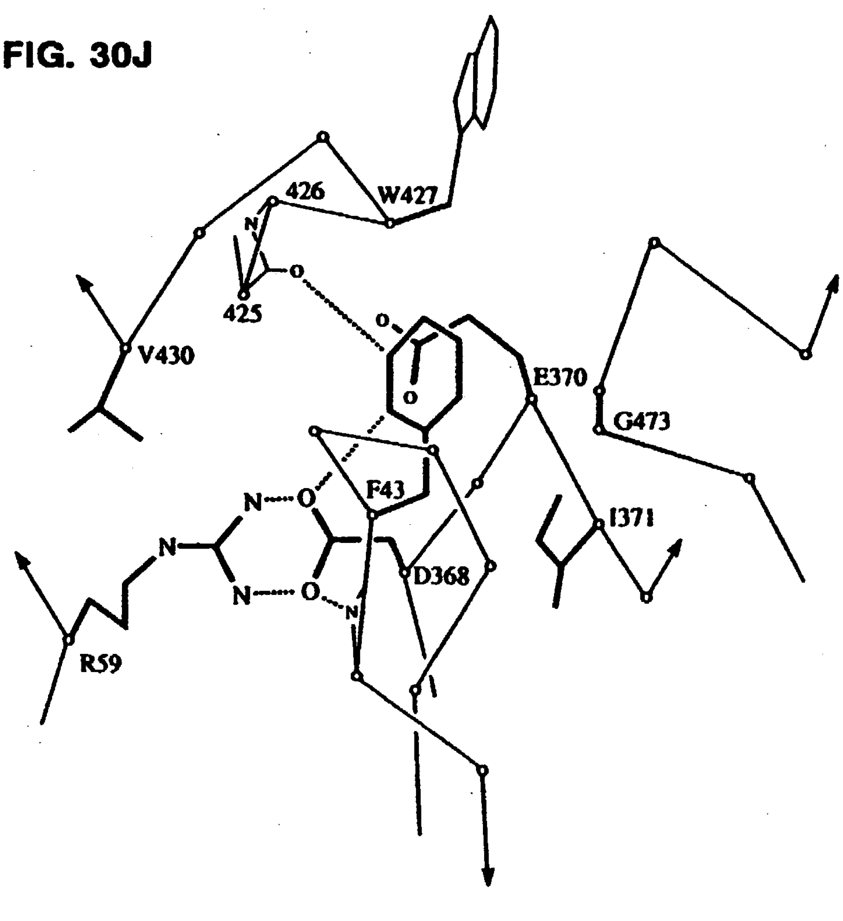


FIG. 31A FIG. 31B

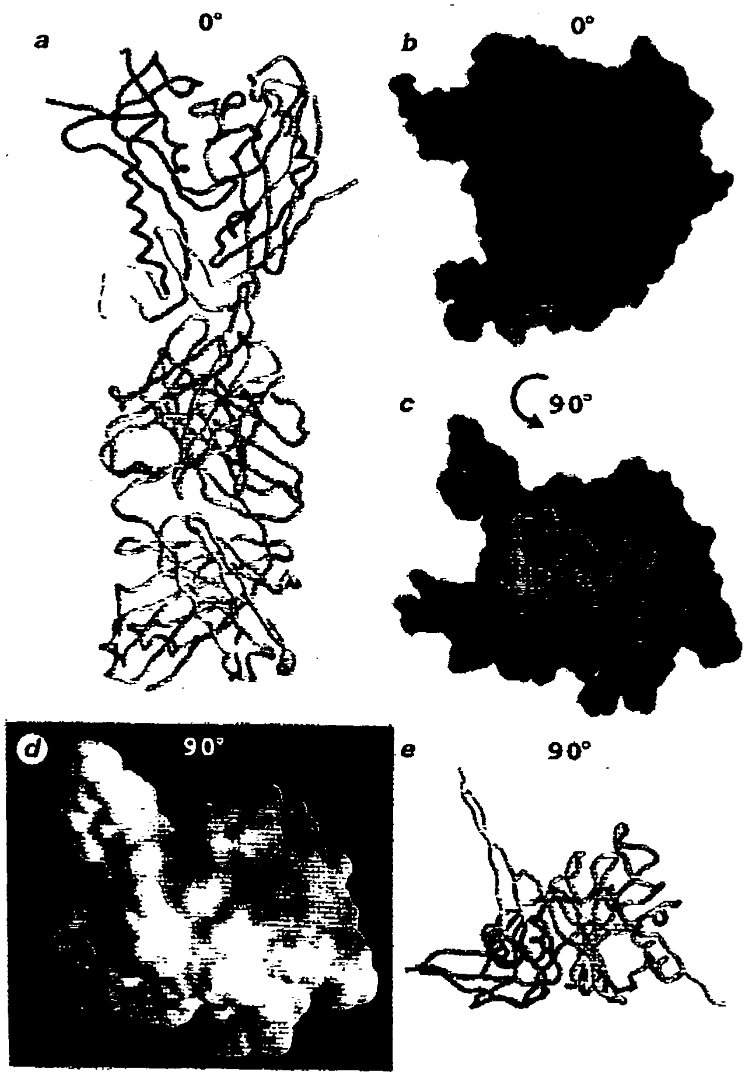


FIG. 31C

FIG. 31D FIG. 31E

FIG. 32

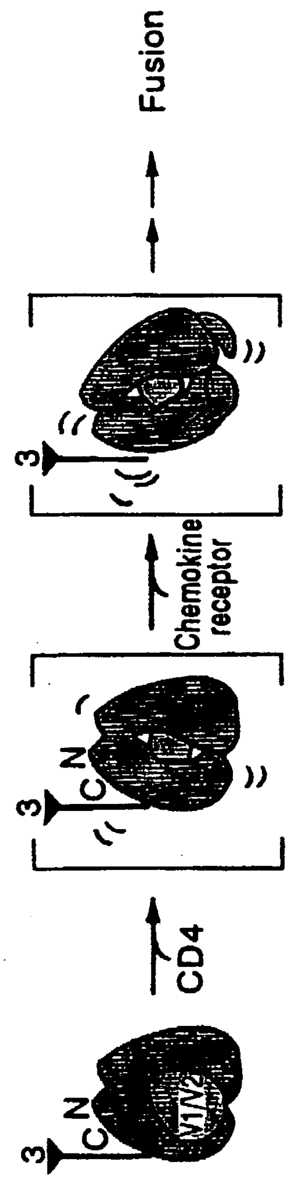


FIG. 33

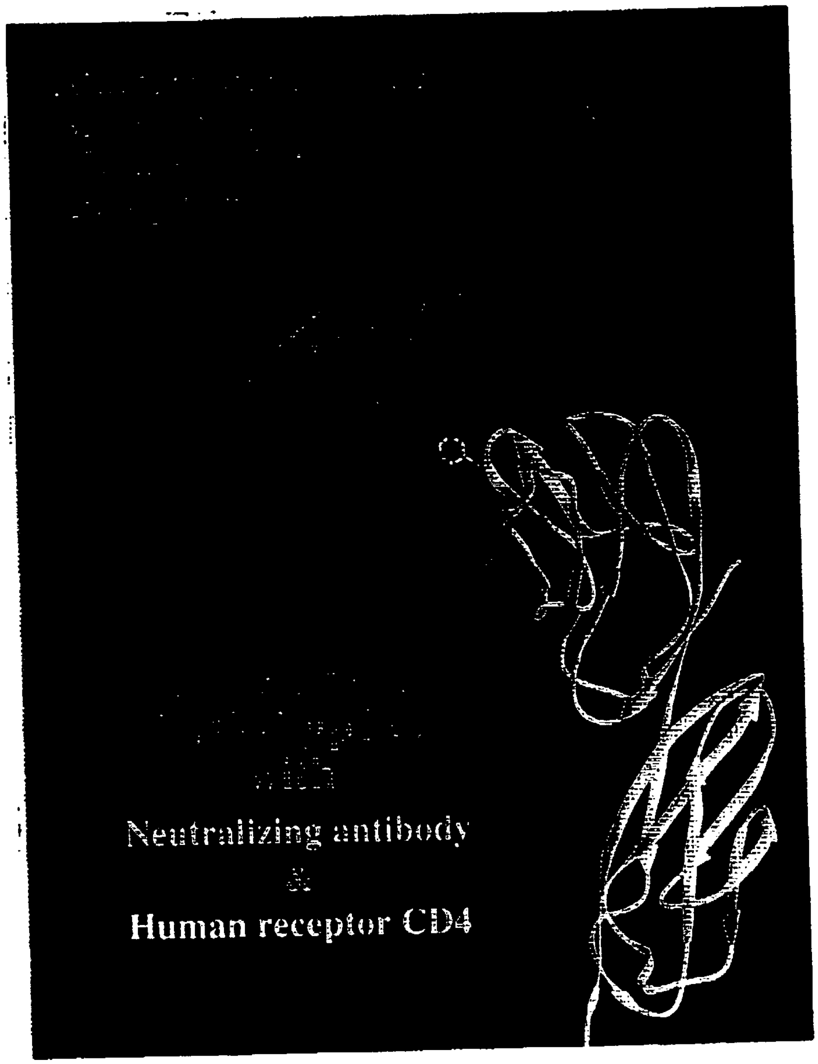


FIG. 34A

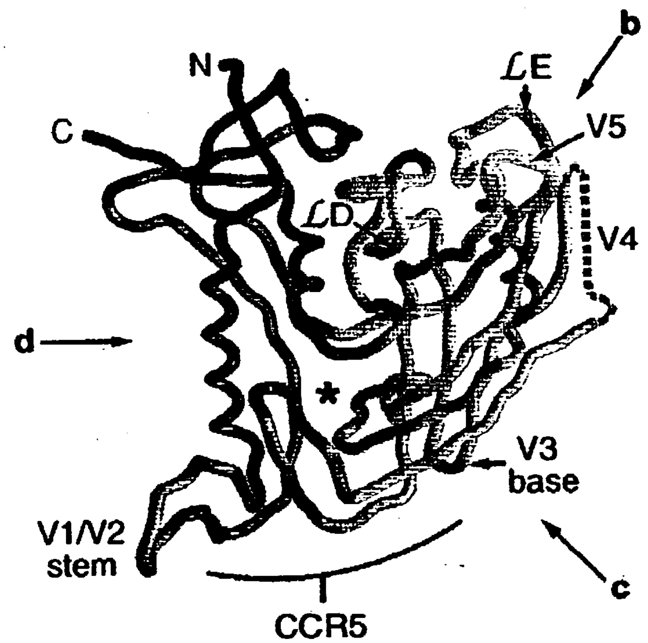


FIG. 34B

FIG. 34C

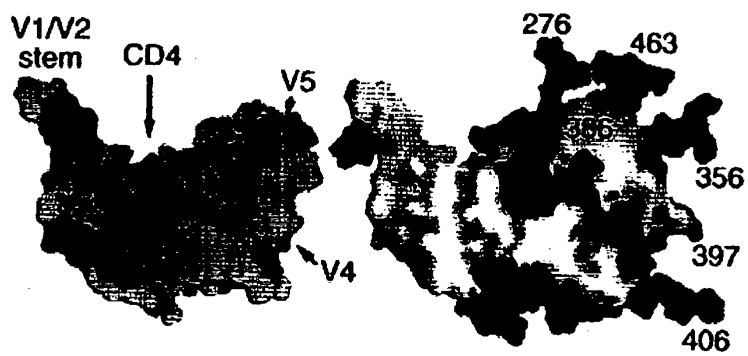


FIG. 34D

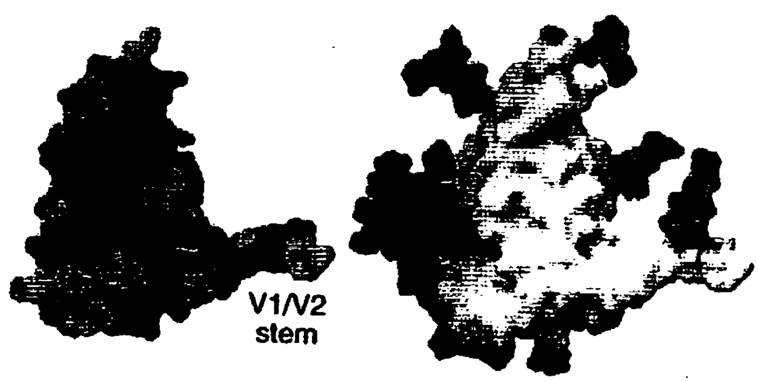


FIG. 35A

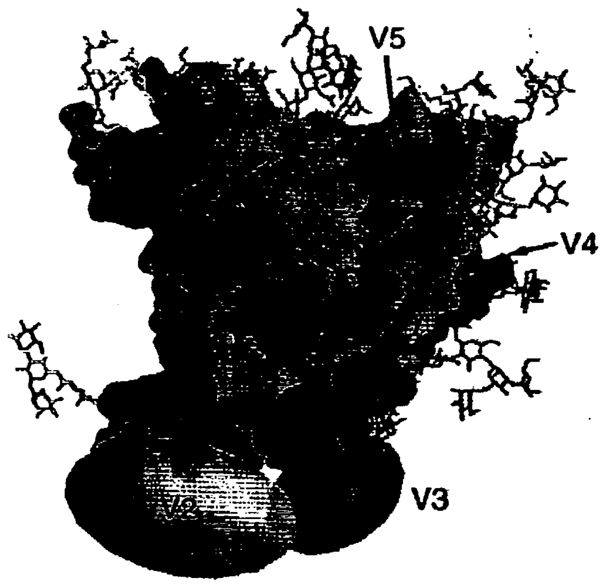


FIG. 35B

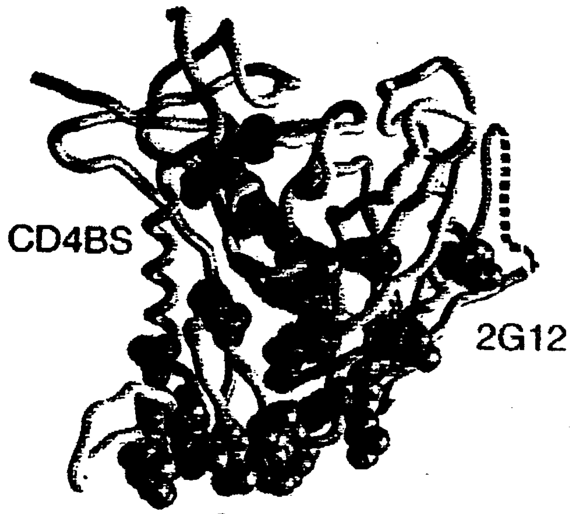


FIG. 35C

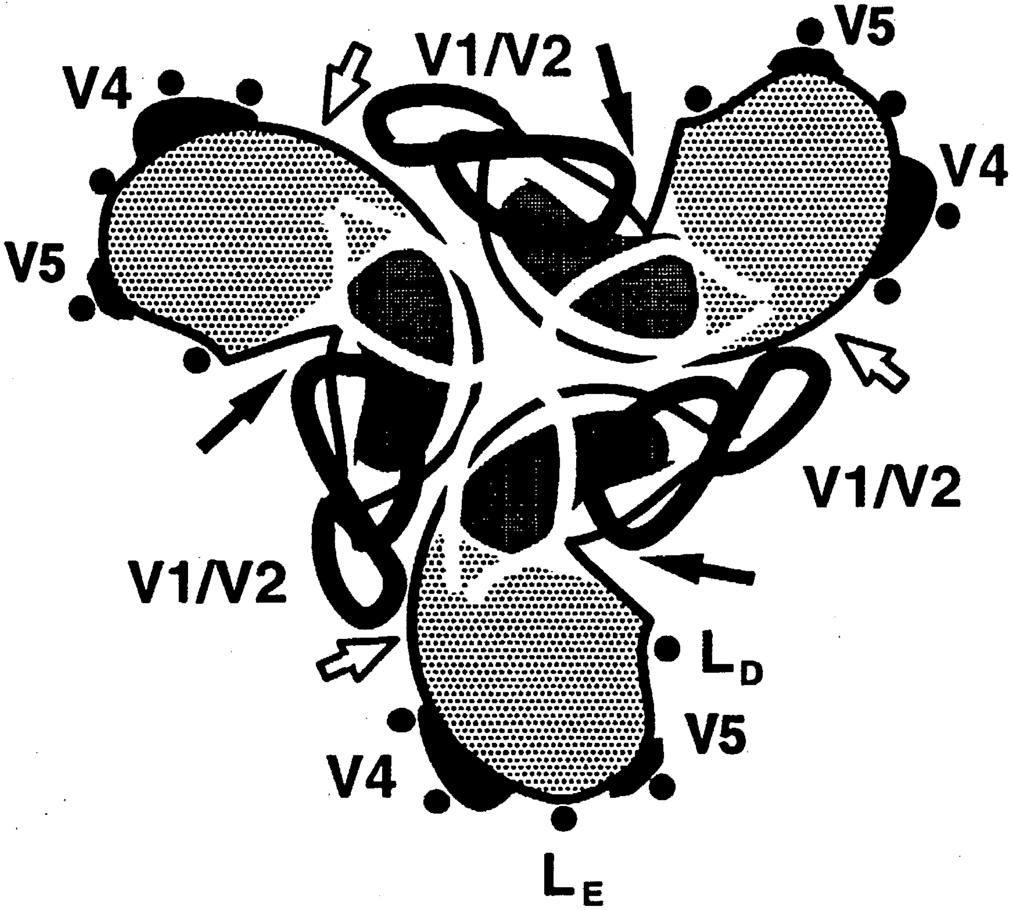


FIG. 35D

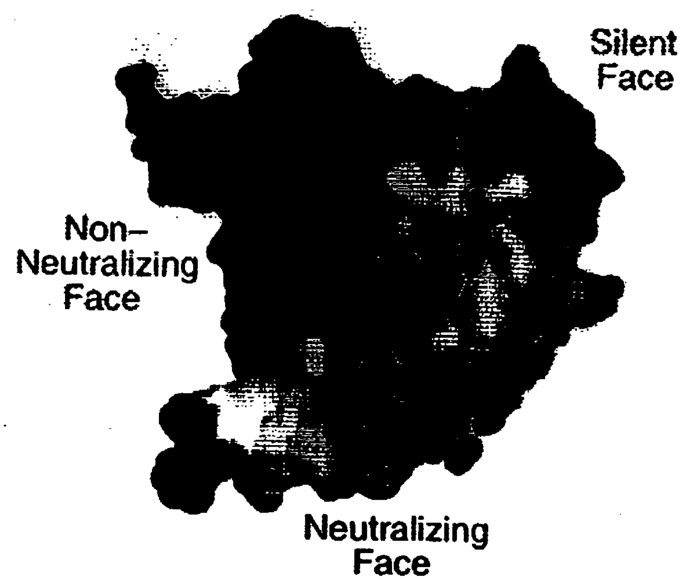
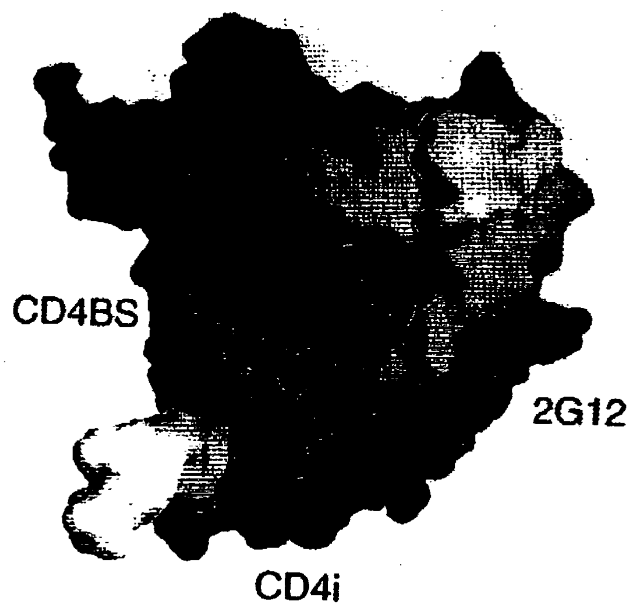


FIG. 36



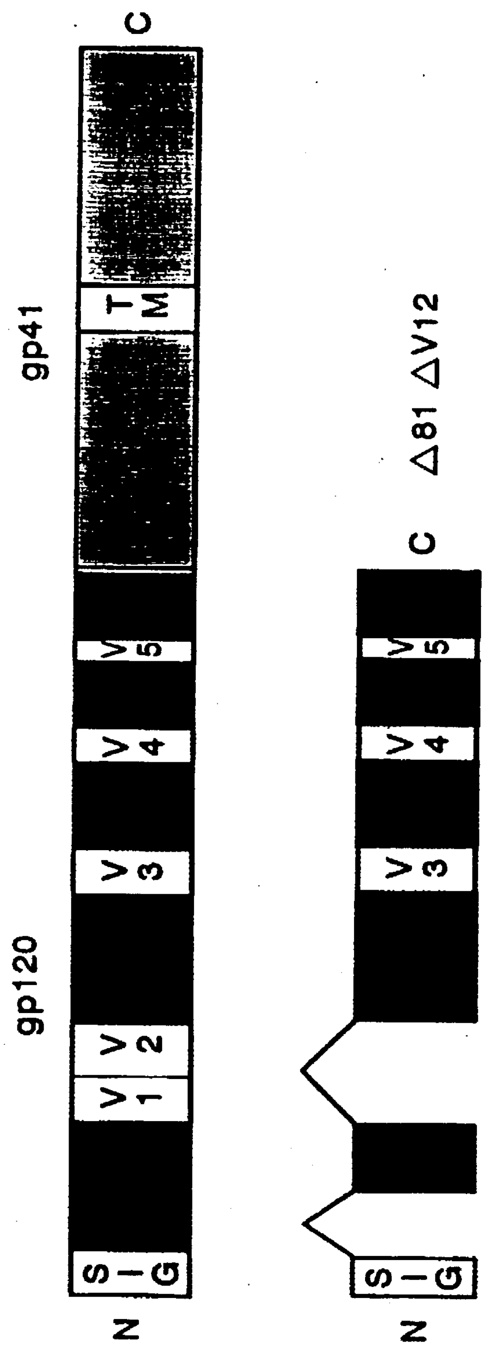


FIG. 37

FIG. 38A

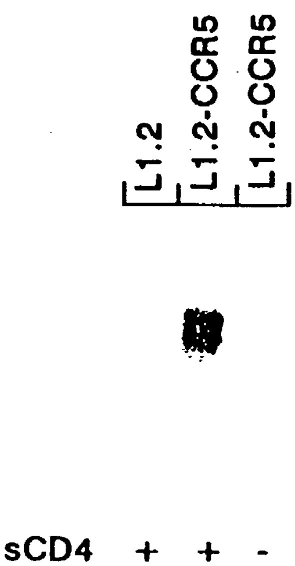


FIG. 38B

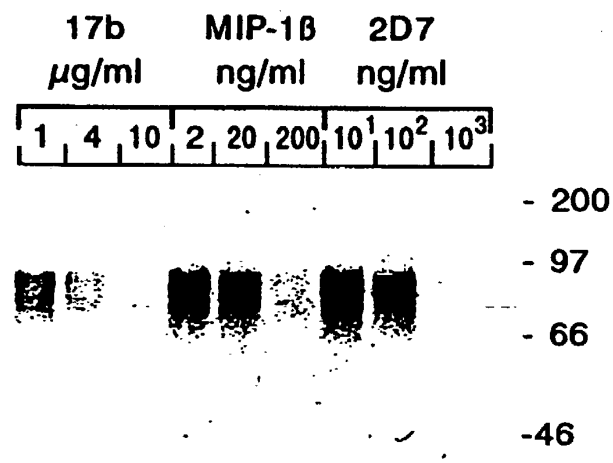


FIG. 38C

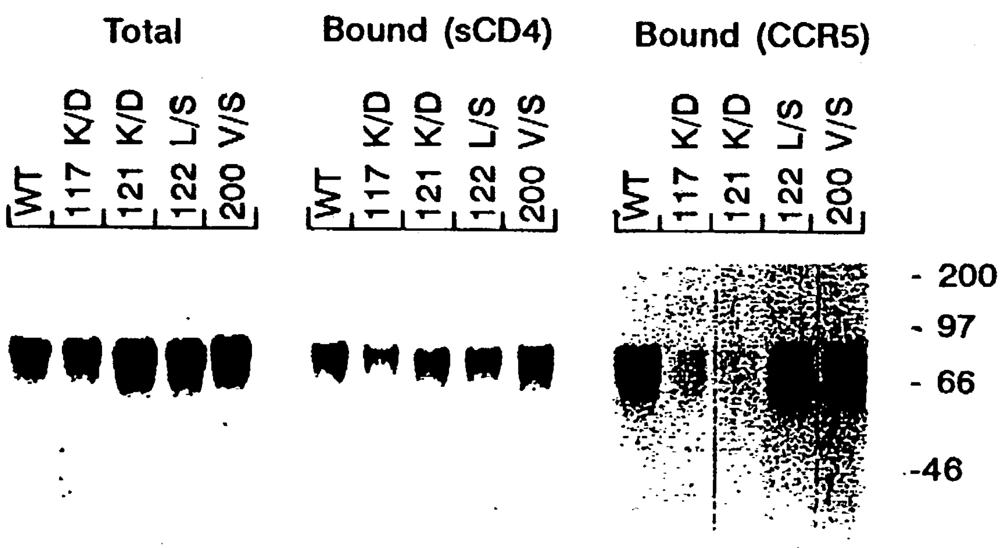


FIG. 39A

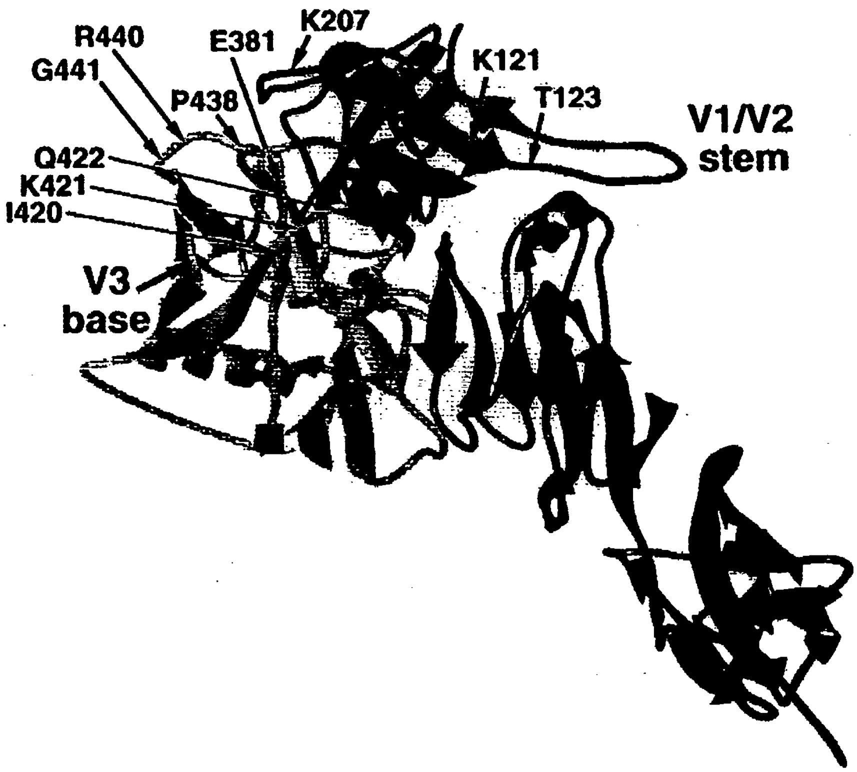

R440
G441
E381
K207
K121
P438
T123
V1/V2
stem
Q422
K421
I420
V3
base

FIG. 39B-1

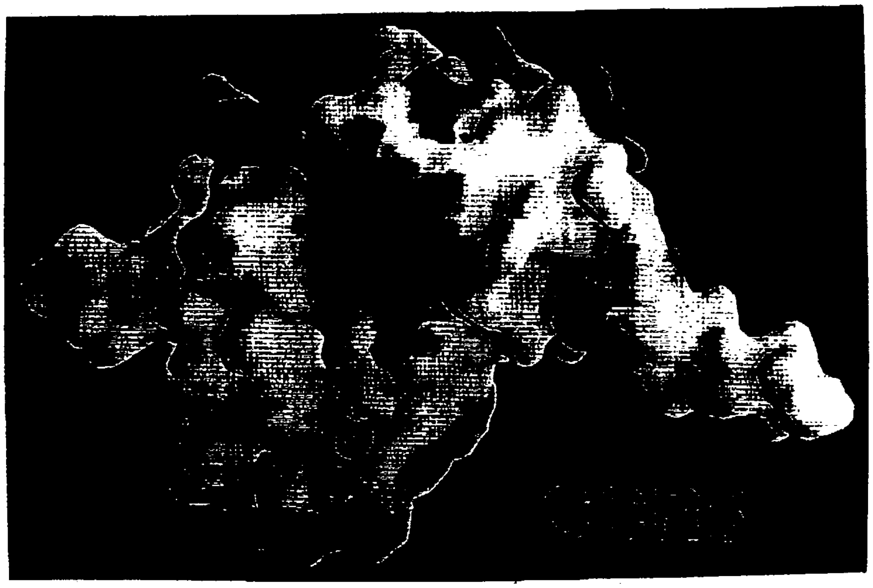


FIG. 39B-2

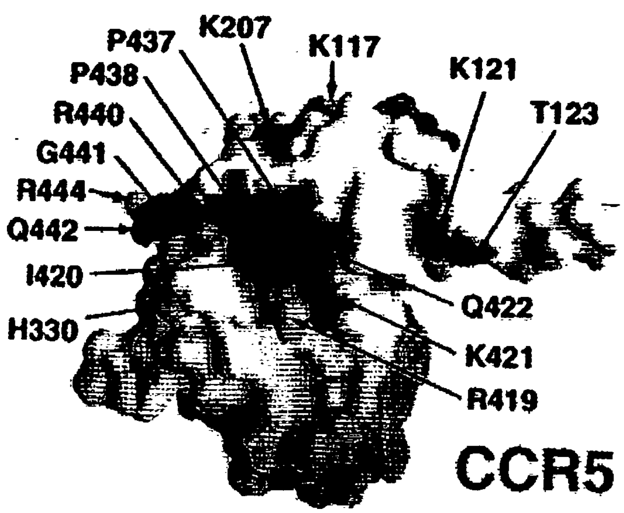


FIG. 39C

FIG. 39D-1

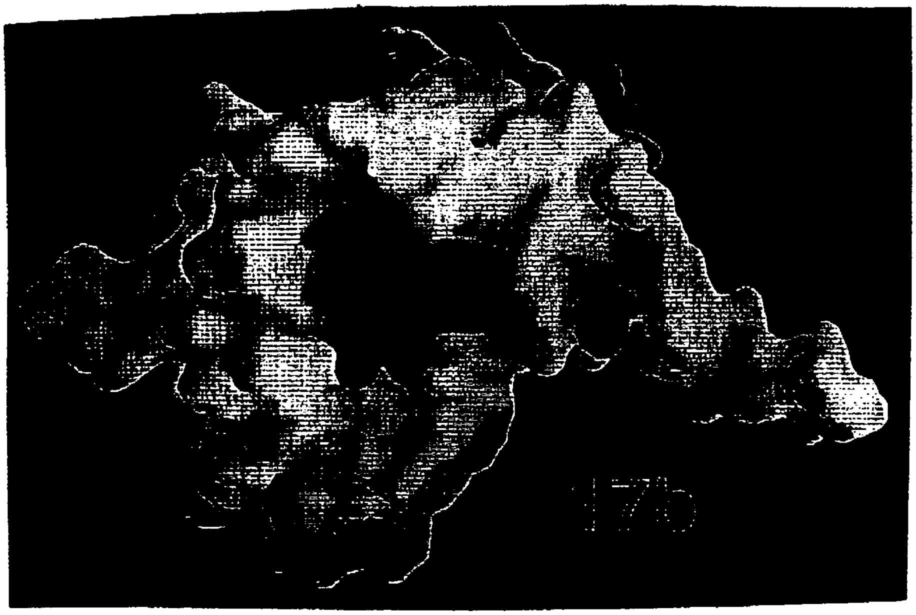


FIG. 39D-2

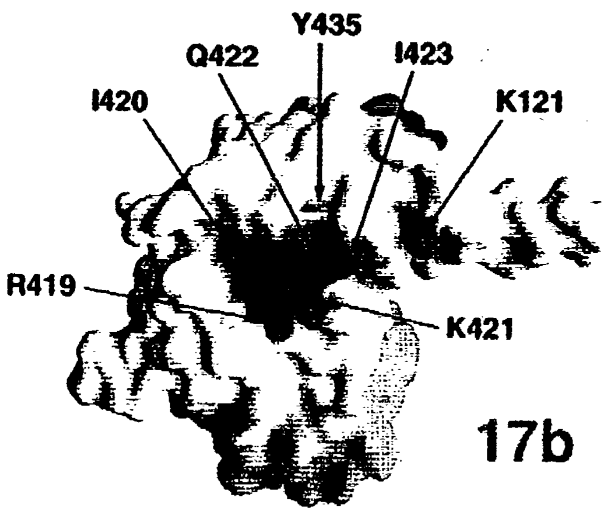


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FIG. 39E-1

FIG. 39E-2

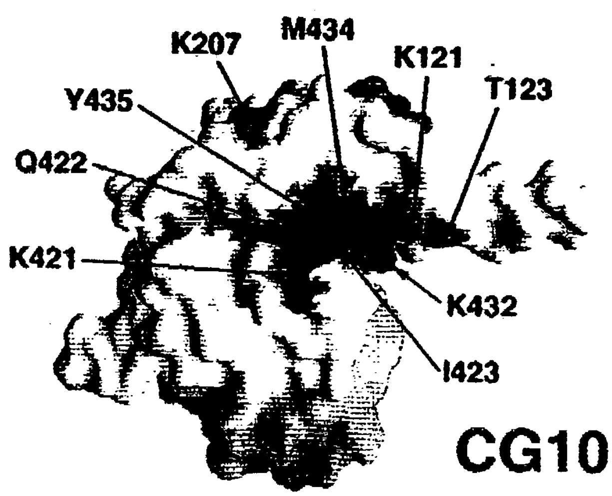


FIG. 40

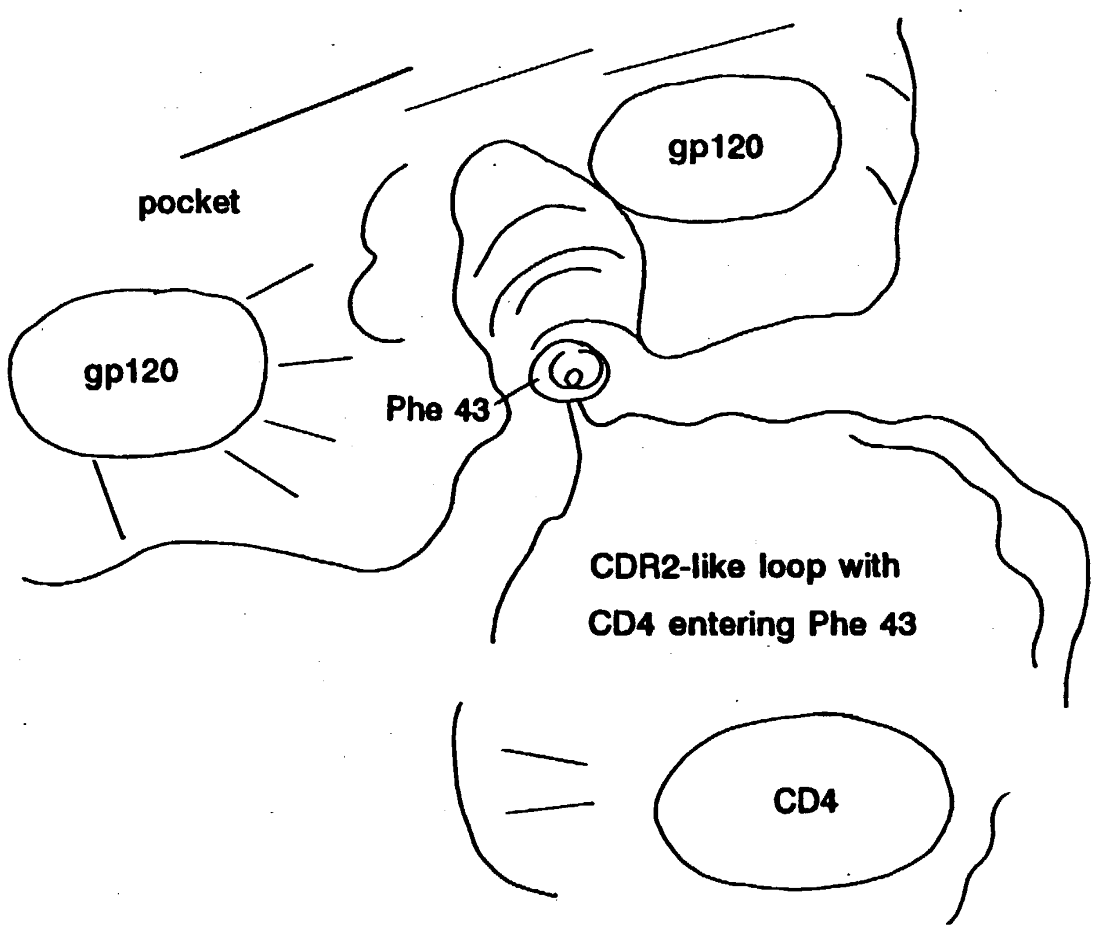

pocket
gp120
gp120
Phe 43
CDR2-like loop with
CD4 entering Phe 43
CD4

FIG. 41A

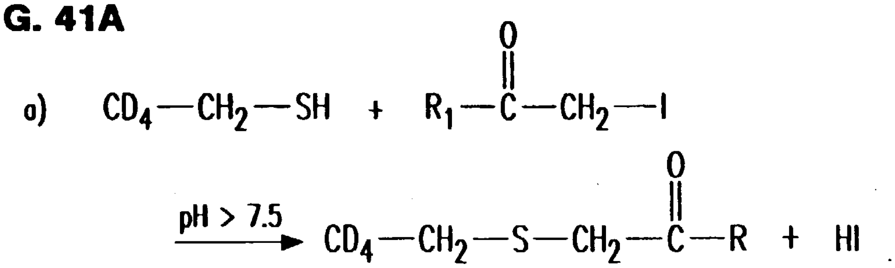


FIG. 41B

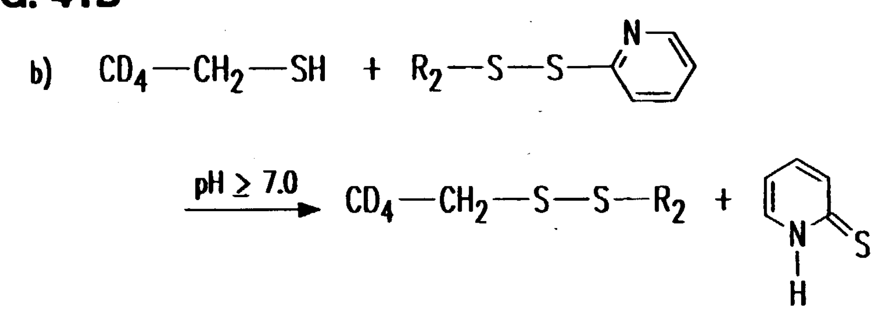
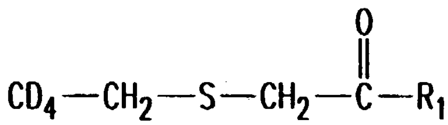


FIG. 42



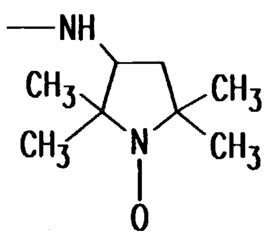
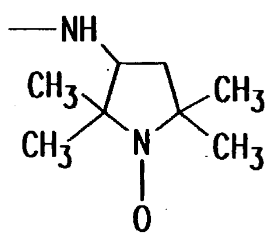
R_1	Reagent
$—NH_2$	Iodoacetamide
	3-(2-Iodoacetamide)-proxyl
	4-(2-Iodoacetamide)-tempo
$—NH—CH_2—CH_2—NHC_{10}H_6SO_3H$	N-Iodoacetyl-N'-(5-sulfonyl-1-naphthyl) ethylene diamine -or- N-Iodoacetyl-N'-(8-sulfonyl-1-naphthyl) ethylene diamine

FIG. 43A

$$AA\text{-}x\text{-}BB + B^{*}\text{-}R_1 \longrightarrow AA\text{-}x\text{-}y\text{-}R_1$$

AA = reactive with thiols
BB = reactive with B*
x = linker
y = result of BB + B*

FIG. 43B

$$CD_4\text{-}CH_2\text{-}SH + AA\text{-}x\text{-}y\text{-}R_1$$

$$\longrightarrow CD_4\text{-}CH_2\text{-}S\text{-}x\text{-}y\text{-}R_1$$

FIG. 44A

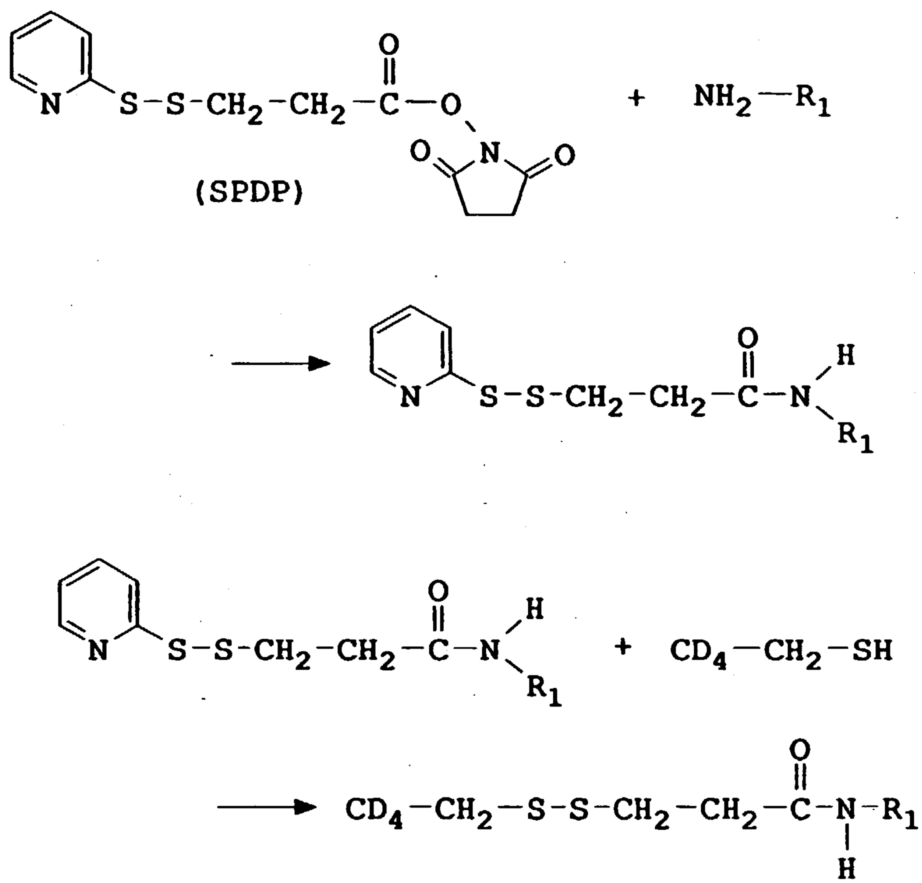

(SPDP)
N
S-S-CH2-CH2-C-O
O
N
O
O
+ NH2—R1
H
R1
+ CD4—CH2—SH
CD4—CH2—S-S-CH2-CH2-C-N-R1

FIG. 44B

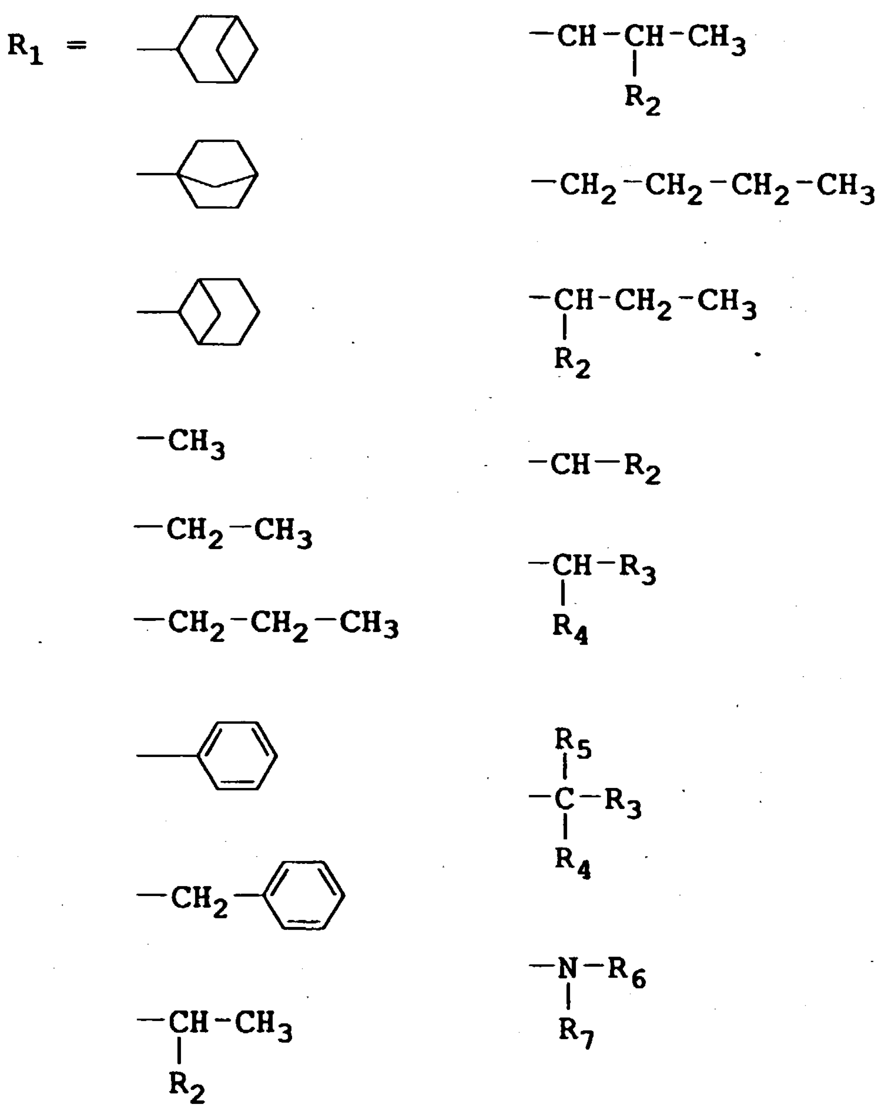

R_1 =
$-CH-CH(R_2)-CH_3$
$-CH_2-CH_2-CH_2-CH_3$
$-CH(R_2)-CH_2-CH_3$
$-CH_3$
$-CH-R_2$
$-CH_2-CH_3$
$-CH(R_4)-R_3$
$-CH_2-CH_2-CH_3$
$-C(R_5)(R_4)-R_3$
$-CH_2-$
$-N(R_7)-R_6$
$-CH(R_2)-CH_3$

FIG. 45

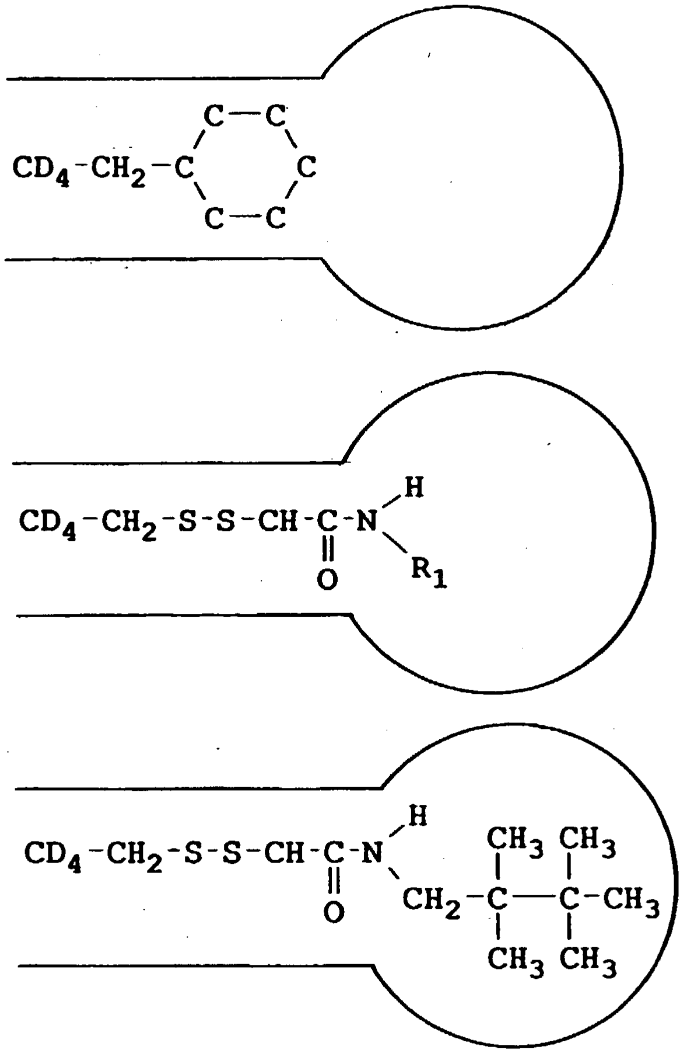

CD4-CH2-C
C—C
C—C
C
CD4-CH2-S-S-CH-C-N
H
R1
O
CD4-CH2-S-S-CH-C-N
H
O
CH2-C—C-CH3
CH3 CH3
CH3 CH3

FIG. 46

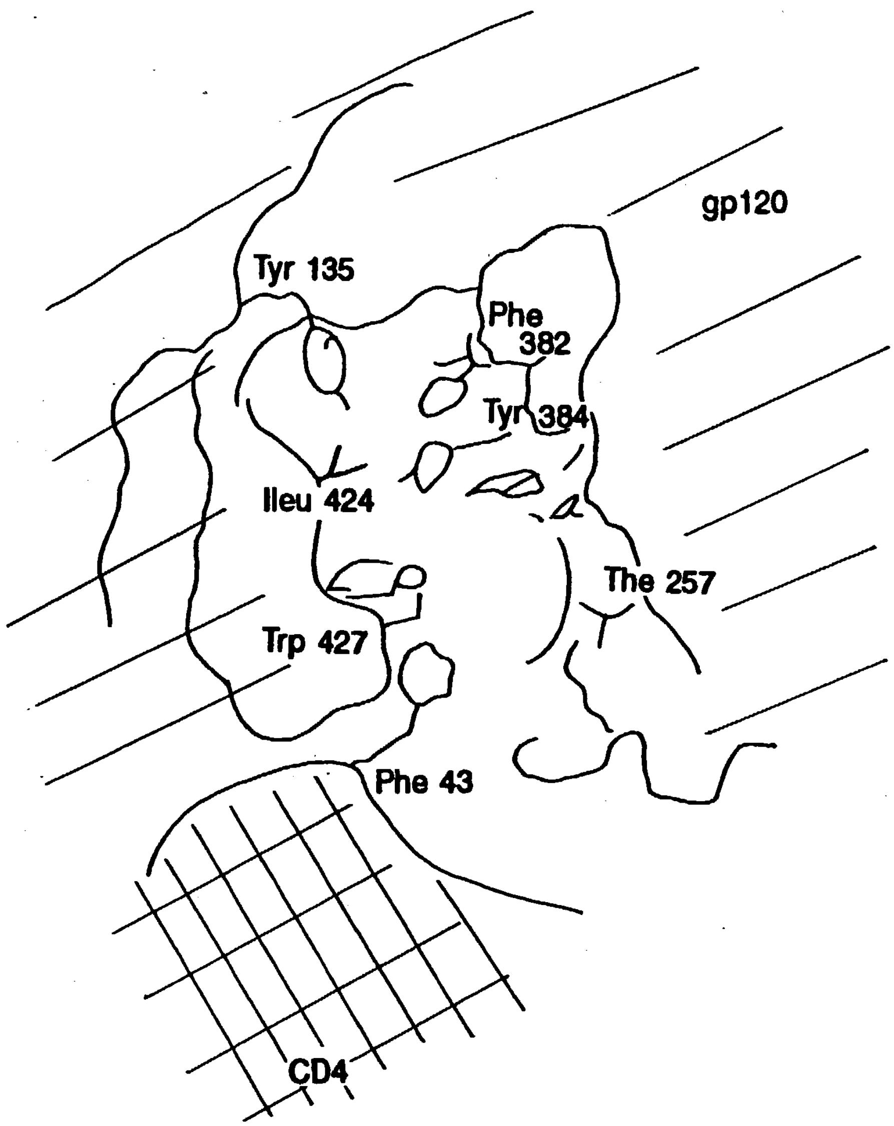
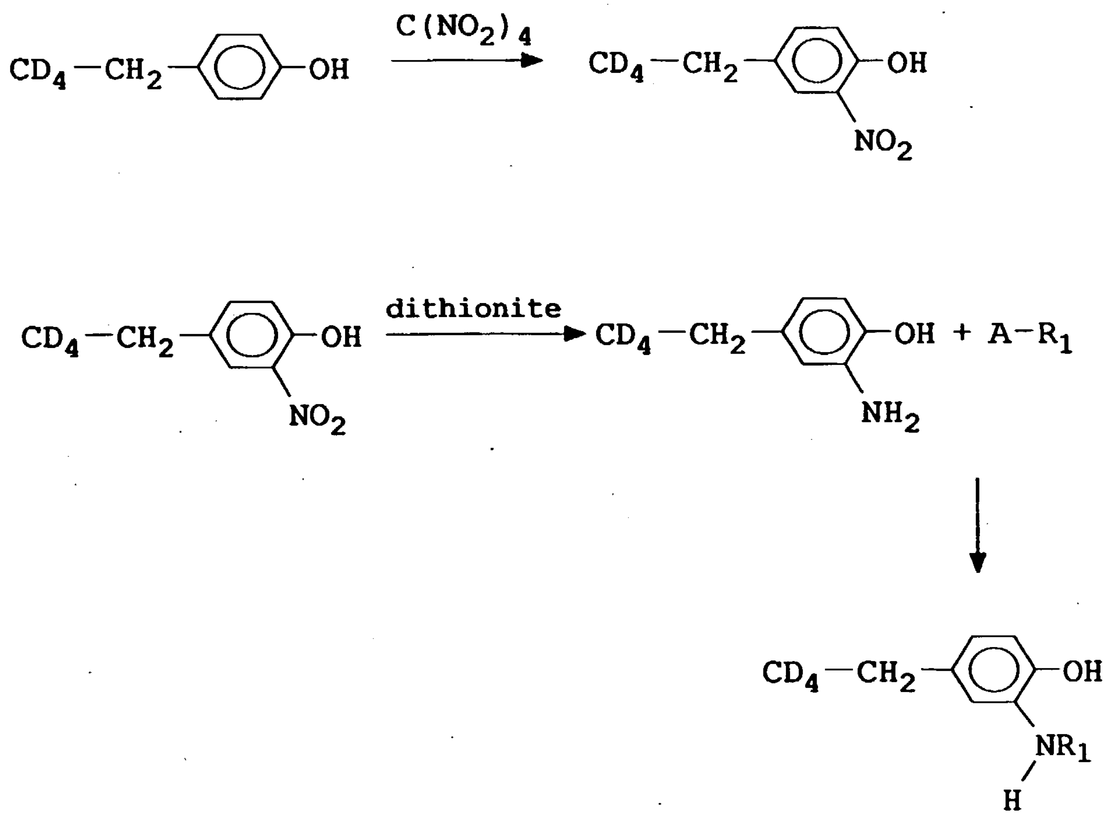

gp120
Tyr 135
Phe
382
Tyr 384
Ileu 424
The 257
Trp 427
Phe 43
CD4

FIG. 47

FIG. 48



09856200.010303

09/856200

66/197

FIG. 49

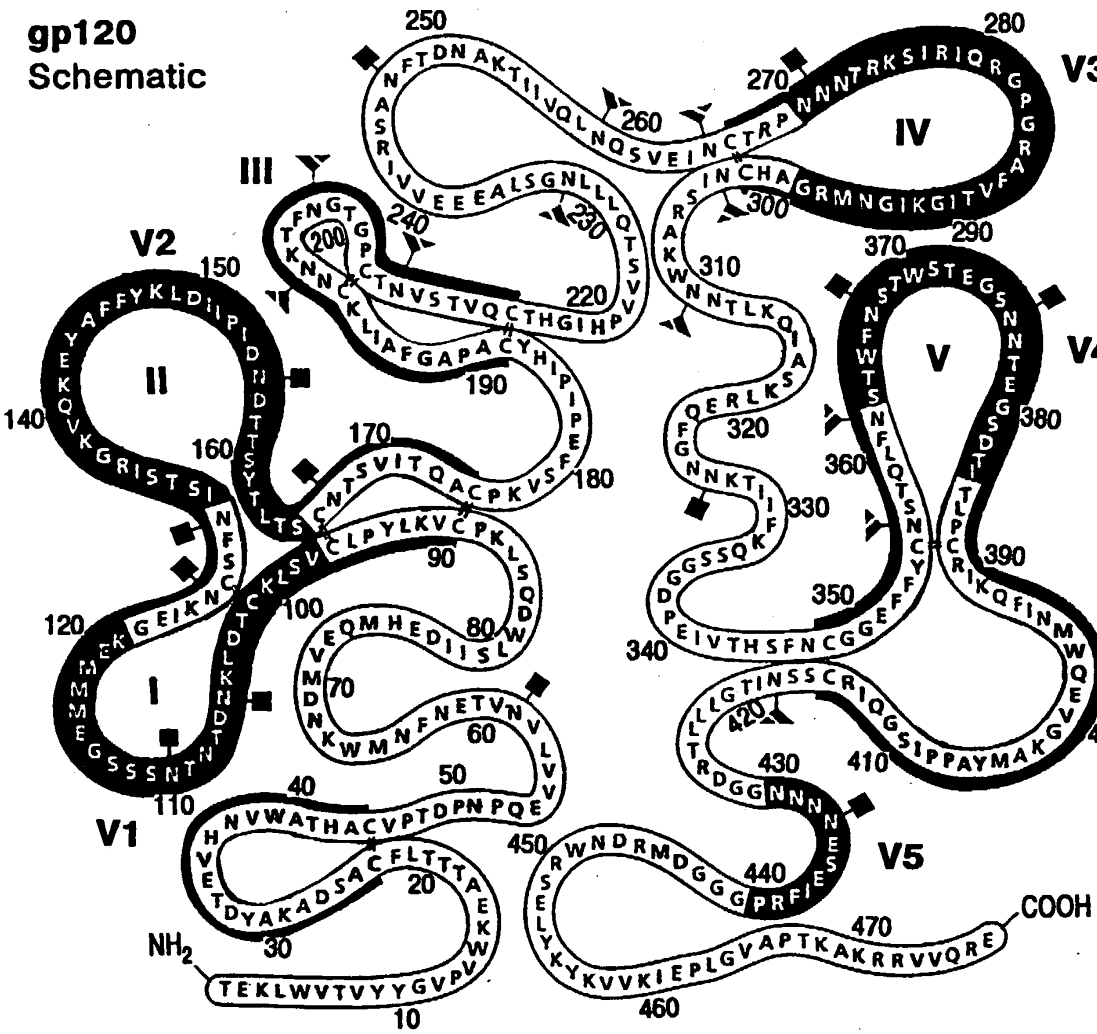


FIG. 50

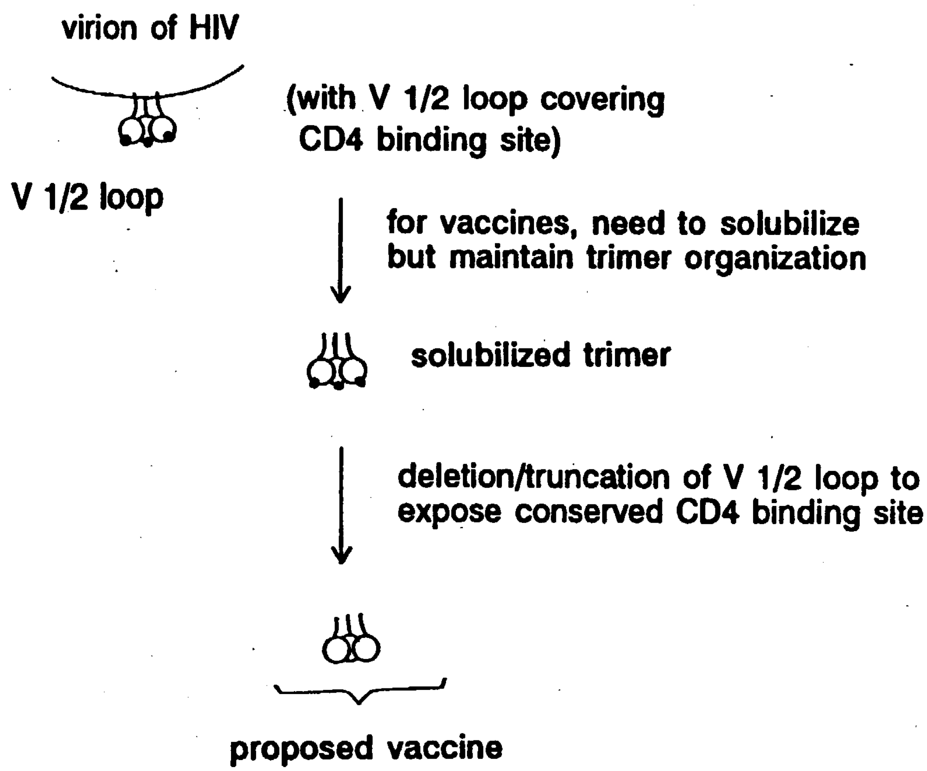
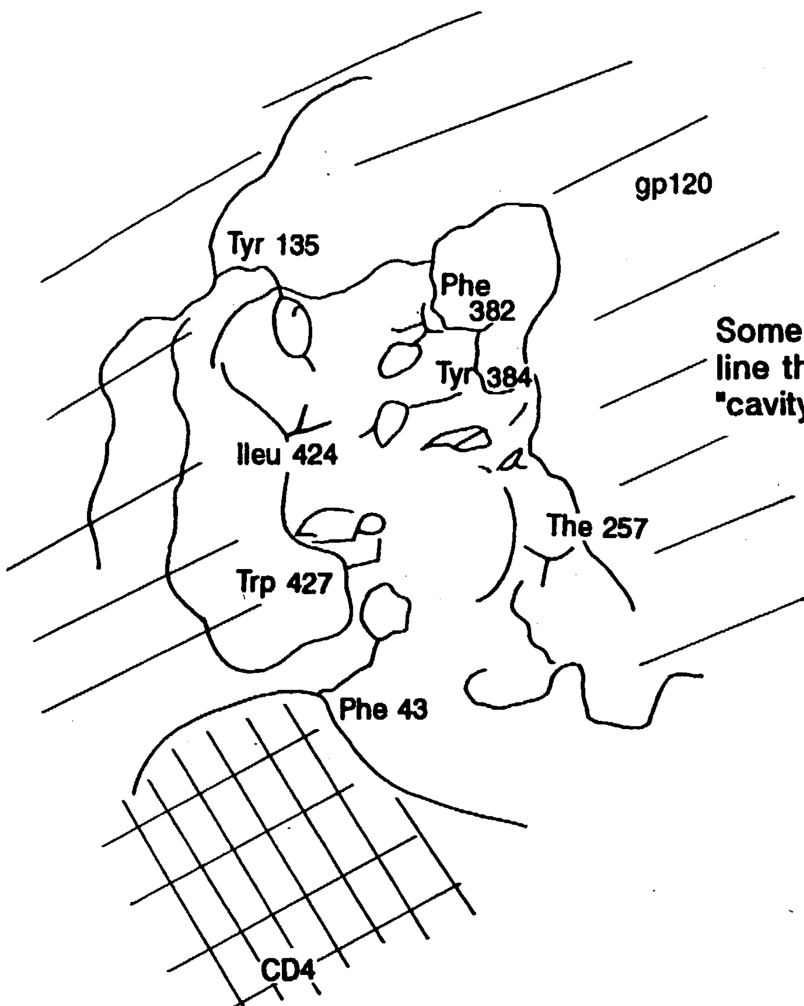

virion of HIV
(with V 1/2 loop covering
CD4 binding site)
V 1/2 loop
for vaccines, need to solubilize
but maintain trimer organization
solubilized trimer
deletion/truncation of V 1/2 loop to
expose conserved CD4 binding site
proposed vaccine

FIG. 51



Some of the residues which line the gp120 "pocket" or "cavity" beyond Phe 43

Residues which line the pocket include:

Trp 112	Ser 375	Asn 428
Leu 116	Asn 377	Ala 433
Pro 118	Phe 382	Gly 473
Phe 210	Ileu 424	Met 475
Val 255	Met 426	
Thr 257	Trp 427	

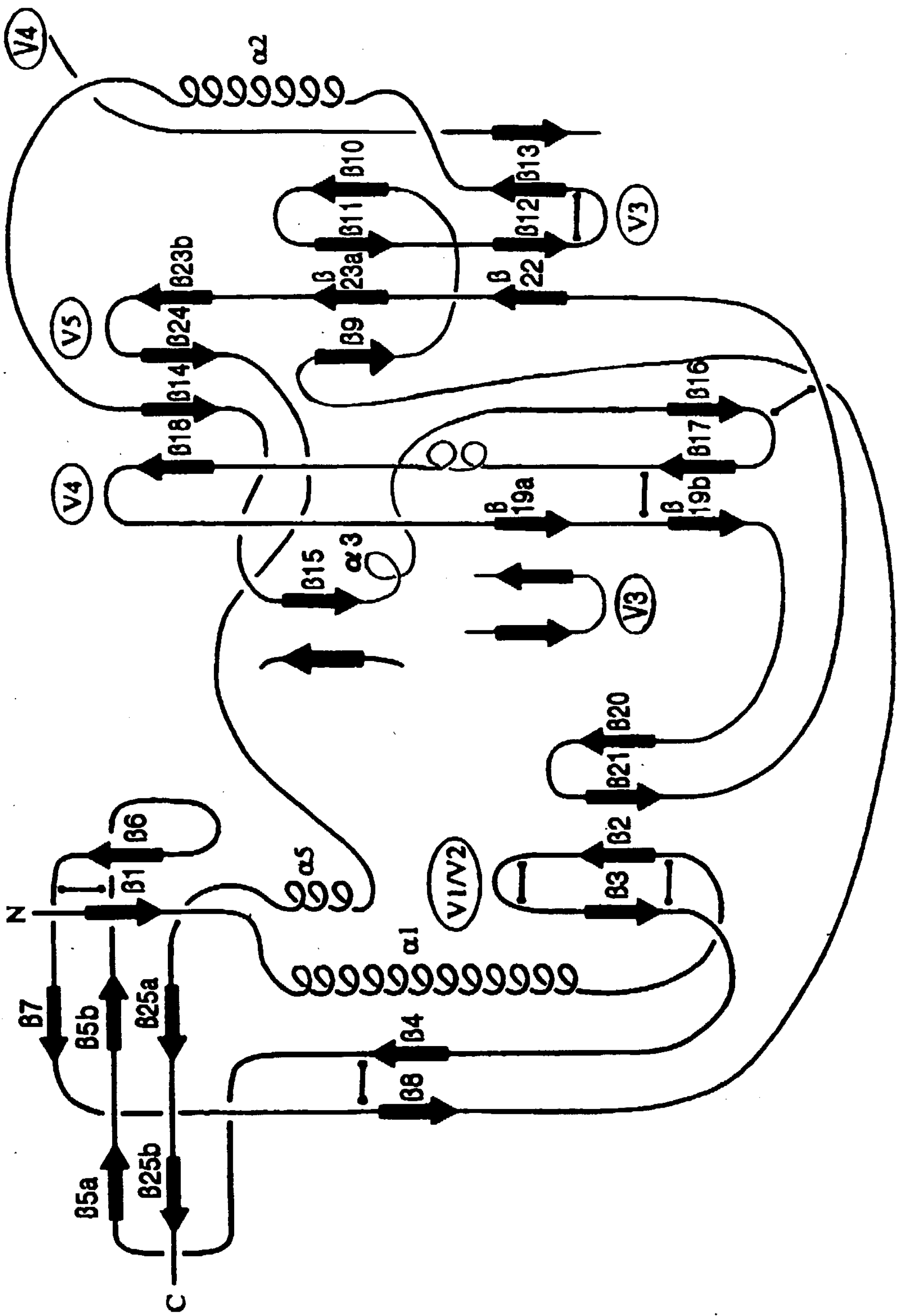

V4
α2
β10
β13
β11
β12
V3
β23b
β 23a
β 22
V5
β24
β9
β14
β16
β18
β17
V4
β 19a
β 19b
β15
α3
V3
β20
β21
β6
β2
α5
V1/V2
N
β1
β3
α1
β7
β5b
β25a
β4
β8
β5a
β25b
C

FIG. 52

FIG. 53-1

```
HEADER    COMPLEX (HIV ENVELOPE PROTEIN/CD4/FAB) 15-JUN-98   1GC1
TITLE     HIV-1 GP120 CORE COMPLEXED WITH CD4 AND A NEUTRALIZING
TITLE    2 HUMAN ANTIBODY
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: ENVELOPE PROTEIN GP120;
COMPND   3 CHAIN: G;
COMPND   4 FRAGMENT: CORE;
COMPND   5 ENGINEERED: YES;
COMPND   6 MUTATION: (GARS) SUBSTITUTION AT THE N TERMINUS, GLY ALA
COMPND   7 GLY SUBSTITUTIONS FOR THE V1/V2 AND V3 LOOPS;
COMPND   8 MOL_ID: 2;
COMPND   9 MOLECULE: CD4;
COMPND  10 CHAIN: C;
COMPND  11 FRAGMENT: D1D2, N-TERMINAL TWO DOMAIN FRAGMENT;
COMPND  12 ENGINEERED: YES;
COMPND  13 MUTATION: S184N, I185T;
COMPND  14 MOL_ID: 3;
COMPND  15 MOLECULE: ANTIBODY 17B;
COMPND  16 CHAIN: L, H;
COMPND  17 FRAGMENT: ANTIGEN-BINDING FRAGMENT, FAB;
COMPND  18 ENGINEERED: YES;
COMPND  19 OTHER_DETAILS: MONOCLONAL ANTIBODY 17B BINDS TO A
COMPND  20 CD4-INDUCED SITE ON GP120
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1;
SOURCE   3 ORGANISM_COMMON: HIV-1;
SOURCE   4 STRAIN: CLADE B;
SOURCE   5 VARIANT: HXBC2;
SOURCE   6 EXPRESSION_SYSTEM: DROSOPHILA MELANOGASTER;
SOURCE   7 OTHER_DETAILS: SECRETED FROM DROSOPHILA SCHNEIDER 2 LINES
SOURCE   8 UNDER_CONTROL OF AN INDUCIBLE METALLOTHIONEIN PROMOTER;
SOURCE   9 MOL_ID: 2;
SOURCE  10 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE  11 ORGANISM_COMMON: HUMAN;
SOURCE  12 EXPRESSION_SYSTEM: CHINESE HAMSTER OVARY CELLS (CHO),
SOURCE  13 CRICETULUS_GRISEUS;
SOURCE  14 MOL_ID: 3;
SOURCE  15 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE  16 ORGANISM_COMMON: HUMAN;
SOURCE  17 EXPRESSION_SYSTEM: EPSTEIN-BARR VIRUS IMMORTALIZED B-CELL
SOURCE  18 CLONE FUSED WITH A MURINE B-CELL FUSION PARTNER
KEYWDS    COMPLEX (HIV ENVELOPE PROTEIN/CD4/FAB), HIV-1 EXTERIOR
KEYWDS   2 ENVELOPE GP120, T-CELL SURFACE GLYCOPROTEIN CD4,
KEYWDS   3 ANTIGEN-BINDING FRAGMENT OF HUMAN IMMUNOGLOBULIN 17B,
KEYWDS   4 GLYCOSYLATED PROTEIN
EXPDTA    X-RAY DIFFRACTION
AUTHOR    P.D.KWONG,R.WYATT,J.ROBINSON,R.W.SWEET,J.SODROSKI,
AUTHOR   2 W.A.HENDRICKSON
REVDAT   2   19-AUG-98 1GC1A   1       SSBOND SOURCE COMPND REMARK
REVDAT   2 1                   1       DBREF  SEQADV
REVDAT   1   08-JUL-98 1GC1    0
JRNL        AUTH   P.D.KWONG,R.WYATT,J.ROBINSON,R.W.SWEET,J.SODROSKI,
JRNL        AUTH 2 W.A.HENDRICKSON
JRNL        TITL   STRUCTURE OF AN HIV GP120 ENVELOPE GLYCOPROTEIN IN
JRNL        TITL 2 COMPLEX WITH THE CD4 RECEPTOR AND A NEUTRALIZING
JRNL        TITL 3 HUMAN ANTIBODY
JRNL        REF    NATURE                         V. 393   648 1998
JRNL        REFN   ASTM NATUAS  UK ISSN 0028-0836                 0006
REMARK   1
REMARK   2
REMARK   2 RESOLUTION. 2.5  ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : X-PLOR 3.8
REMARK   3   AUTHORS     : BRUNGER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.5
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 5
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 2
```

FIG. 53-2

```
REMARK  3   DATA CUTOFF LOW         (ABS(F)) : 0.1
REMARK  3   COMPLETENESS (WORKING+TEST)   (%) : 74.9
REMARK  3   NUMBER OF REFLECTIONS             : 28620
REMARK  3
REMARK  3  FIT TO DATA USED IN REFINEMENT.
REMARK  3   CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK  3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK  3   R VALUE            (WORKING SET) : 0.2103
REMARK  3   FREE R VALUE                     : 0.3026
REMARK  3   FREE R VALUE TEST SET SIZE   (%) : 5
REMARK  3   FREE R VALUE TEST SET COUNT      : 1430
REMARK  3   ESTIMATED ERROR OF FREE R VALUE  : NULL
REMARK  3
REMARK  3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK  3   TOTAL NUMBER OF BINS USED           : 10
REMARK  3   BIN RESOLUTION RANGE HIGH       (A) : 2.50
REMARK  3   BIN RESOLUTION RANGE LOW        (A) : 2.58
REMARK  3   BIN COMPLETENESS (WORKING+TEST) (%) : 42.3
REMARK  3   REFLECTIONS IN BIN    (WORKING SET) : 1518
REMARK  3   BIN R VALUE           (WORKING SET) : 0.2876
REMARK  3   BIN FREE R VALUE                    : 0.3878
REMARK  3   BIN FREE R VALUE TEST SET SIZE  (%) : 5.7
REMARK  3   BIN FREE R VALUE TEST SET COUNT     : 92
REMARK  3   ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK  3
REMARK  3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK  3   PROTEIN ATOMS            : 7080
REMARK  3   NUCLEIC ACID ATOMS       : 0
REMARK  3   HETEROGEN ATOMS          : 194
REMARK  3   SOLVENT ATOMS            : 602
REMARK  3
REMARK  3  B VALUES.
REMARK  3   FROM WILSON PLOT           (A**2) : NULL
REMARK  3   MEAN B VALUE      (OVERALL, A**2) : 21
REMARK  3   OVERALL ANISOTROPIC B VALUE.
REMARK  3    B11 (A**2) : 0
REMARK  3    B22 (A**2) : 0
REMARK  3    B33 (A**2) : 0
REMARK  3    B12 (A**2) : 0
REMARK  3    B13 (A**2) : 0
REMARK  3    B23 (A**2) : 0
REMARK  3
REMARK  3  ESTIMATED COORDINATE ERROR.
REMARK  3   ESD FROM LUZZATI PLOT        (A) : NULL
REMARK  3   ESD FROM SIGMAA              (A) : NULL
REMARK  3   LOW RESOLUTION CUTOFF        (A) : 5.0
REMARK  3
REMARK  3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK  3   ESD FROM C-V LUZZATI PLOT    (A) : NULL
REMARK  3   ESD FROM C-V SIGMAA          (A) : NULL
REMARK  3
REMARK  3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK  3   BOND LENGTHS                 (A) : 0.007
REMARK  3   BOND ANGLES            (DEGREES) : 1.59
REMARK  3   DIHEDRAL ANGLES        (DEGREES) : NULL
REMARK  3   IMPROPER ANGLES        (DEGREES) : NULL
REMARK  3
REMARK  3  ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK  3
REMARK  3  ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS    SIGMA
REMARK  3   MAIN-CHAIN BOND              (A**2) : 1.33  ; 1.0
REMARK  3   MAIN-CHAIN ANGLE             (A**2) : 2.31  ; 1.5
REMARK  3   SIDE-CHAIN BOND              (A**2) : 1.97  ; 1.5
REMARK  3   SIDE-CHAIN ANGLE             (A**2) : 3.01  ; 2.0
REMARK  3
REMARK  3  NCS MODEL : NULL
REMARK  3
REMARK  3  NCS RESTRAINTS.                     RMS   SIGMA/WEIGHT
REMARK  3   GROUP  1  POSITIONAL          (A) : NULL  ; NULL
REMARK  3   GROUP  1  B-FACTOR         (A**2) : NULL  ; NULL
```

FIG. 53-3

```
REMARK   3 PARAMETER FILE  1  : PARAM3_MOD.CHO
REMARK   3 PARAMETER FILE  2  : PARAMCSDX.MISC
REMARK   3 PARAMETER FILE  3  : PARAMCSDX_MOD.PRO
REMARK   3 PARAMETER FILE  4  : PARAM19.SOL
REMARK   3 TOPOLOGY FILE  1   : TOPHCSDX.PRO
REMARK   3 TOPOLOGY FILE  2   : TOPH3.CHO
REMARK   3 TOPOLOGY FILE  3   : TOPHCSDX.MISC
REMARK   3
REMARK   3 OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 1GC1 COMPLIES WITH FORMAT V. 2.2, 16-DEC-1996
REMARK   6
REMARK   6 RESIDUES 83-89 AND 397-409 OF GP120 AND 182-185 OF CD4 ARE
REMARK   6 DISORDERED AND ARE IN SEQUENCE LIST BUT NOT IN ATOMS LIST.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        ; AUG-1996
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 7.0
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : NSLS
REMARK 200  BEAMLINE                       : X4A
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 1.00614
REMARK 200  MONOCHROMATOR                  : SILICON CRYSTAL
REMARK 200  OPTICS                         : MIRRORS
REMARK 200
REMARK 200  DETECTOR TYPE                  : PHOSPHOR IMAGE PLATE
REMARK 200   FUJI BAS2000 SCANNER
REMARK 200  DETECTOR MANUFACTURER          : FUJI
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200  DATA SCALING SOFTWARE          : SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 37724
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.5
REMARK 200  RESOLUTION RANGE LOW       (A) : 20.
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : -0.5
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 86
REMARK 200  DATA REDUNDANCY                : 3.0
REMARK 200  R MERGE                    (I) : NULL
REMARK 200  R SYM                      (I) : 0.093
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 9.17
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.50
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.59
REMARK 200  COMPLETENESS FOR SHELL     (%) : 62.8
REMARK 200  DATA REDUNDANCY IN SHELL       : 1.56
REMARK 200  R MERGE FOR SHELL          (I) : NULL
REMARK 200  R SYM FOR SHELL            (I) : 0.247
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 2.17
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: NULL
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR
REMARK 200   REPLACEMENT + MULTIPLE ISOMORPHOUS REPLACEMENT + DENSITY
REMARK 200   MODIFICATION
REMARK 200 SOFTWARE USED: MERLOT, AMORE, MLPHARE, DM, PRISM
REMARK 200 STARTING MODEL: PDB ENTRIES 1HIL, 1CDH AND 3CD4
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 59
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.00
```

FIG. 53-4

```
REMARK 280 CRYSTALLIZATION CONDITIONS: VAPOUR DIFFUSION
REMARK 280 CRYSTALLIZATION: 0.5 UL OF PROTEIN
REMARK 280 (~10MG/ML IN 350 MM NACL, 5 MM TRISCL PH 7.0) + 0.4 UL OF
REMARK 280 0.1 M NACITRATE, 0.02 M NAHEPES, 10% ISOPROPANOL, 10.5%
REMARK 280 MONOMETHYL-PEG 5000, 0.0075% SEAPREP AGAROSE, PH 6.4 OVER
REMARK 280 A RESERVOIR OF 0.35 M NACL, 0.1 M NACITRATE, 0.02 M
REMARK 280 NAHEPES, 10% ISOPROPANOL, 10.5% MONOMETHYL-PEG 5000,
REMARK 280 PH 6.4
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 2 2 21
REMARK 290
REMARK 290    SYMOP  SYMMETRY
REMARK 290   NNNMMM  OPERATOR
REMARK 290     1555  X,Y,Z
REMARK 290     2555  -X,-Y,1/2+Z
REMARK 290     3555  -X,Y,1/2-Z
REMARK 290     4555  X,-Y,-Z
REMARK 290
REMARK 290   WHERE NNN -> OPERATOR NUMBER
REMARK 290         MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1  1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2  1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3  1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1  2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2  2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3  2  0.000000  0.000000  1.000000       98.34776
REMARK 290   SMTRY1  3 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2  3  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3  3  0.000000  0.000000 -1.000000       98.34776
REMARK 290   SMTRY1  4  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2  4  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3  4  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 650
REMARK 650 HELIX
REMARK 650 DETERMINATION METHOD: AUTHOR-DETERMINED + KABSCH AND SANDER
REMARK 650  ALGORITHM
REMARK 700
REMARK 700 SHEET
REMARK 700 DETERMINATION METHOD: AUTHOR-DETERMINED + KABSCH AND SANDER
REMARK 700  ALGORITHM
REMARK 700 SHEET G CONTAINS INTERMOLECULAR HYDROGEN BONDING
REMARK 700  (STRAND #15 OF CORE GP120 TO STRAND C" OF CD4).
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: O
REMARK 800 SITE_DESCRIPTION: WATER HOH 1000 (ZERO OCCUPANCY) MARKS
REMARK 800  THE LOCATION OF THE CENTRAL UNMODELLED DENSITY IN THE
REMARK 800  "PHE 43" CAVITY.
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 1GC1 G   SWS    P04578     1 -   89 NOT IN ATOMS LIST
REMARK 999 1GC1 G   SWS    P04578   397 -  409 NOT IN ATOMS LIST
REMARK 999 1GC1 G   SWS    P04578   493 -  856 NOT IN ATOMS LIST
REMARK 999 1GC1 C   SWS    P01730     1 -   25 NOT IN ATOMS LIST
REMARK 999 1GC1 C   SWS    P01730   207 -  458 NOT IN ATOMS LIST
REMARK 999
REMARK 999 REFERENCE: THE INSERTED RESIDUES GARS AT THE N-TERMINUS OF
REMARK 999 THE GP120 SEQUENCE AND NT AT THE C-TERMINUS OF CD4 ARE
REMARK 999 CLONING ARTIFACTS.  GP120: G 128, A 129, G 194 SUBSTITUTE
REMARK 999 FOR THE V1/V2 LOOP (128-194), G 298, A 299, G 329
REMARK 999 SUBSTITUTE FOR V3 LOOP (298-329).
REMARK 999
```

FIG. 53-5

```
REMARK 999 BEEN CORRECTED IN THIS PDB ENTRY: D94N, D346A, L470P.
REMARK 999 THE 17B ANTIBODY SEQUENCE WAS DETERMINED DURING THE COURSE
REMARK 999 OF THE STRUCTURE DETERMINATION AND HAS NOT YET BEEN
REMARK 999 DEPOSITED IN ANY SEQUENCE DATA BANK (PERSONAL
REMARK 999 COMMUNICATION, RICHARD WYATT).
DBREF 1GC1 G 90 127 SWS P04578 ENV_HV1H2 90 127
DBREF 1GC1 G 128 194 PDB 1GC1 1GC1 128 194
DBREF 1GC1 G 195 297 SWS P04578 ENV_HV1H2 195 297
DBREF 1GC1 G 298 329 PDB 1GC1 1GC1 298 329
DBREF 1GC1 G 330 396 SWS P04578 ENV_HV1H2 330 396
DBREF 1GC1 G 410 492 SWS P04578 ENV_HV1H2 410 492
DBREF 1GC1 C 1 181 SWS P01730 CD4_HUMAN 26 206
DBREF 1GC1 L 1 213 PDB 1GC1 1GC1 1 213
DBREF 1GC1 H 1 229 PDB 1GC1 1GC1 1 229
SEQADV 1GC1 ASN G 94 SWS P04578 ASP 94 CONFLICT
SEQADV 1GC1 ALA G 346 SWS P04578 ASP 346 CONFLICT
SEQADV 1GC1 G SWS P04578 ASN 397 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 SER 398 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 THR 399 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 TRP 400 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 SER 401 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 THR 402 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 GLU 403 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 GLY 404 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 SER 405 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 ASN 406 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 ASN 407 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 THR 408 GAP IN PDB ENTRY
SEQADV 1GC1 G SWS P04578 GLU 409 GAP IN PDB ENTRY
SEQADV 1GC1 PRO G 470 SWS P04578 LEU 470 CONFLICT
SEQRES 1 G 321 GLY ALA ARG SER GLU VAL VAL LEU VAL ASN VAL THR GLU
SEQRES 2 G 321 ASN PHE ASN MET TRP LYS ASN ASP MET VAL GLU GLN MET
SEQRES 3 G 321 HIS GLU ASP ILE ILE SER LEU TRP ASP GLN SER LEU LYS
SEQRES 4 G 321 PRO CYS VAL LYS LEU THR PRO LEU CYS VAL GLY ALA GLY
SEQRES 5 G 321 SER CYS ASN THR SER VAL ILE THR GLN ALA CYS PRO LYS
SEQRES 6 G 321 VAL SER PHE GLU PRO ILE PRO ILE HIS TYR CYS ALA PRO
SEQRES 7 G 321 ALA GLY PHE ALA ILE LEU LYS CYS ASN ASN LYS THR PHE
SEQRES 8 G 321 ASN GLY THR GLY PRO CYS THR ASN VAL SER THR VAL GLN
SEQRES 9 G 321 CYS THR HIS GLY ILE ARG PRO VAL VAL SER THR GLN LEU
SEQRES 10 G 321 LEU LEU ASN GLY SER LEU ALA GLU GLU GLU VAL VAL ILE
SEQRES 11 G 321 ARG SER VAL ASN PHE THR ASP ASN ALA LYS THR ILE ILE
SEQRES 12 G 321 VAL GLN LEU ASN THR SER VAL GLU ILE ASN CYS THR GLY
SEQRES 13 G 321 ALA GLY HIS CYS ASN ILE SER ARG ALA LYS TRP ASN ASN
SEQRES 14 G 321 THR LEU LYS GLN ILE ALA SER LYS LEU ARG GLU GLN PHE
SEQRES 15 G 321 GLY ASN ASN LYS THR ILE ILE PHE LYS GLN SER SER GLY
SEQRES 16 G 321 GLY ASP PRO GLU ILE VAL THR HIS SER PHE ASN CYS GLY
SEQRES 17 G 321 GLY GLU PHE PHE TYR CYS ASN SER THR GLN LEU PHE ASN
SEQRES 18 G 321 SER THR TRP PHE ASN SER THR TRP SER THR LYS GLY SER
SEQRES 19 G 321 ASN ASN THR GLU GLY SER ASP THR ILE THR LEU PRO CYS
SEQRES 20 G 321 ARG ILE LYS GLN ILE ILE ASN MET TRP GLN LYS VAL GLY
SEQRES 21 G 321 LYS ALA MET TYR ALA PRO PRO ILE SER GLY GLN ILE ARG
SEQRES 22 G 321 CYS SER SER ASN ILE THR GLY LEU LEU LEU THR ARG ASP
SEQRES 23 G 321 GLY GLY ASN SER ASN ASN GLU SER GLU ILE PHE ARG PRO
SEQRES 24 G 321 GLY GLY GLY ASP MET ARG ASP ASN TRP ARG SER GLU LEU
SEQRES 25 G 321 TYR LYS TYR LYS VAL VAL LYS ILE GLU
SEQRES 1 C 185 LYS LYS VAL VAL LEU GLY LYS LYS GLY ASP THR VAL GLU
SEQRES 2 C 185 LEU THR CYS THR ALA SER GLN LYS LYS SER ILE GLN PHE
SEQRES 3 C 185 HIS TRP LYS ASN SER ASN GLN ILE LYS ILE LEU GLY ASN
SEQRES 4 C 185 GLN GLY SER PHE LEU THR LYS GLY PRO SER LYS LEU ASN
SEQRES 5 C 185 ASP ARG ALA ASP SER ARG ARG SER LEU TRP ASP GLN GLY
SEQRES 6 C 185 ASN PHE PRO LEU ILE ILE LYS ASN LEU LYS ILE GLU ASP
SEQRES 7 C 185 SER ASP THR TYR ILE CYS GLU VAL GLU ASP GLN LYS GLU
SEQRES 8 C 185 GLU VAL GLN LEU LEU VAL PHE GLY LEU THR ALA ASN SER
SEQRES 9 C 185 ASP THR HIS LEU LEU GLN GLY GLN SER LEU THR LEU THR
SEQRES 10 C 185 LEU GLU SER PRO PRO GLY SER SER PRO SER VAL GLN CYS
SEQRES 11 C 185 ARG SER PRO ARG GLY LYS ASN ILE GLN GLY GLY LYS THR
SEQRES 12 C 185 LEU SER VAL SER GLN LEU GLU LEU GLN ASP SER GLY THR
SEQRES 13 C 185 TRP THR CYS THR VAL LEU GLN ASN GLN LYS LYS VAL GLU
SEQRES 14 C 185 PHE LYS ILE ASP ILE VAL VAL LEU ALA PHE GLN LYS ALA
SEQRES 15 C 185 SER ASN THR
```

FIG. 53-6

```
SEQRES  2 L 213  SER PRO GLY GLU ARG ALA THR LEU SER CYS ARG ALA SER
SEQRES  3 L 213  GLU SER VAL SER SER ASP LEU ALA TRP TYR GLN GLN LYS
SEQRES  4 L 213  PRO GLY GLN ALA PRO ARG LEU LEU ILE TYR GLY ALA SER
SEQRES  5 L 213  THR ARG ALA THR GLY VAL PRO ALA ARG PHE SER GLY SER
SEQRES  6 L 213  GLY SER GLY ALA GLU PHE THR LEU THR ILE SER SER LEU
SEQRES  7 L 213  GLN SER GLU ASP PHE ALA VAL TYR TYR CYS GLN GLN TYR
SEQRES  8 L 213  ASN ASN TRP PRO PRO ARG TYR THR PHE GLY GLN GLY THR
SEQRES  9 L 213  ARG LEU GLU ILE LYS ARG THR VAL ALA ALA PRO SER VAL
SEQRES 10 L 213  PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY
SEQRES 11 L 213  THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO
SEQRES 12 L 213  ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU
SEQRES 13 L 213  GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP
SEQRES 14 L 213  SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR
SEQRES 15 L 213  LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA
SEQRES 16 L 213  CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR
SEQRES 17 L 213  LYS SER PHE ASN ARG
SEQRES  1 H 229  GLN VAL GLN LEU LEU GLU SER GLY ALA GLU VAL LYS LYS
SEQRES  2 H 229  PRO GLY SER SER VAL LYS VAL SER CYS LYS ALA SER GLY
SEQRES  3 H 229  ASP THR PHE ILE ARG TYR SER PHE THR TRP VAL ARG GLN
SEQRES  4 H 229  ALA PRO GLY GLN GLY LEU GLU TRP MET GLY ARG ILE ILE
SEQRES  5 H 229  THR ILE LEU ASP VAL ALA HIS TYR ALA PRO HIS LEU GLN
SEQRES  6 H 229  GLY ARG VAL THR ILE THR ALA ASP LYS SER THR SER THR
SEQRES  7 H 229  VAL TYR LEU GLU LEU ARG ASN LEU ARG SER ASP ASP THR
SEQRES  8 H 229  ALA VAL TYR PHE CYS ALA GLY VAL TYR GLU GLY GLU ALA
SEQRES  9 H 229  ASP GLU GLY GLU TYR ASP ASN ASN GLY PHE LEU LYS HIS
SEQRES 10 H 229  TRP GLY GLN GLY THR LEU VAL THR VAL THR SER ALA SER
SEQRES 11 H 229  THR LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER
SEQRES 12 H 229  LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU
SEQRES 13 H 229  VAL LYS ASP TYR PHE PRO GLN PRO VAL THR VAL SER TRP
SEQRES 14 H 229  ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO
SEQRES 15 H 229  ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER
SEQRES 16 H 229  VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR
SEQRES 17 H 229  TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS
SEQRES 18 H 229  VAL ASP LYS LYS VAL GLU PRO LYS
HET    NAG  G 697      14
HET    NAG  G 734      14
HET    NAG  G 762      14
HET    NAG  G 776      14
HET    NAG  G 789      14
HET    NAG  G 795      14
HET    NAG  G 832      14
HET    NAG  G 839      14
HET    NAG  G 886      14
HET    NAG  G 892      14
HET    NAG  G 948      14
HET    FUC  G 735      10
HET    FUC  G 796      10
HET    FUC  G 893      10
HET    FUC  G 949      10
HETNAM     NAG N-ACETYL-D-GLUCOSAMINE
HETNAM     FUC FUCOSE
FORMUL   5  NAG    11(C8 H15 N1 O6)
FORMUL   6  FUC    4(C6 H12 O5)
FORMUL   7  HOH   *603(H2 O1)
HELIX    1 GA1 MET G  100  LEU G  116  1                                  17
HELIX    2 GA2 ARG G  335  SER G  347  1                                  13
HELIX    3 GA3 ASP G  368  THR G  373  1                                   6
HELIX    4 GA4 THR G  388  PHE G  391  5 SLIGHTLY NON-STANDARD             4
HELIX    5 GA5 MET G  475  TYR G  484  1                                  10
HELIX    6 CA1 ARG C   58  GLY C   65  5 IRREGULAR                         8
HELIX    7 CA2 LYS C   75  SER C   79  5                                   5
HELIX    8 CA3 GLU C  150  SER C  154  5                                   5
HELIX    9 LA1 SER L  123  GLY L  130  1                                   8
HELIX   10 LA2 LYS L  185  GLU L  189  1                                   5
HELIX   11 HA1 THR H   28  ILE H   30  5                                   3
HELIX   12 HA2 ARG H   87  THR H   91  5                                   5
HELIX   13 HA3 SER H  171  ALA H  173  5                                   3
SHEET    1   A 2 ASN G  92  ASN G  94  0
SHEET    2   A 2 GLY G 237  CYS G 239 -1
SHEET    1   B 4 SER G 199  ILE G 201  0
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FIG. 53-7

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SHEET 3 B 4 VAL G 430 TYR G 435 -1
SHEET 4 B 4 GLN G 422 MET G 426 -1
SHEET 1 C 1 PRO G 214 ALA G 219 0
SHEET 2 C 2 GLN G 246 ILE G 251 -1
SHEET 1 D 3 ASN G 241 VAL G 245 0
SHEET 2 D 3 GLY G 222 ASN G 229 -1
SHEET 3 D 3 LYS G 485 ILE G 491 -1
SHEET 1 E 7 LEU G 261 GLY G 263 0
SHEET 2 E 7 ILE G 443 ILE G 449 1
SHEET 3 E 7 VAL G 292 GLY G 298 -1
SHEET 4 E 7 GLY G 329 SER G 334 -1
SHEET 5 E 7 ASP G 412 LYS G 421 -1
SHEET 6 E 7 GLU G 381 ASN G 386 -1
SHEET 7 E 7 HIS G 374 CYS G 378 -1
SHEET 1 F 6 VAL G 271 ARG G 273 0
SHEET 2 F 6 ILE G 284 LEU G 288 -1
SHEET 3 F 6 THR G 450 ASP G 457 -1
SHEET 4 F 6 GLU G 464 GLY G 471 -1
SHEET 5 F 6 THR G 358 LYS G 362 1
SHEET 6 F 6 SER G 393 TRP G 395 -1
SHEET 1 G 7 LYS C 2 LYS C 7 0
SHEET 2 G 7 GLN C 89 PHE C 98 1 N GLN C 94 O LYS C 2
SHEET 3 G 7 ASP C 80 VAL C 86 -1 N VAL C 86 O GLN C 89
SHEET 4 G 7 HIS C 27 LYS C 29 -1 N LYS C 29 O ILE C 83
SHEET 5 G 7 LYS C 35 GLN C 40 -1 N LEU C 37 O TRP C 28
SHEET 6 G 7 PHE C 43 LYS C 46 -1 N THR C 45 O GLY C 38
SHEET 7 G 7 GLY G 366 GLY G 367 -1 N GLY G 367 O LEU C 44
SHEET 1 H 2 VAL C 12 LEU C 14 0
SHEET 2 H 2 LEU C 69 ILE C 71 -1 N ILE C 71 O VAL C 12
SHEET 1 I 3 GLY C 99 ALA C 102 0
SHEET 2 I 3 LEU C 114 GLU C 119 -1 N GLU C 119 O GLY C 99
SHEET 3 I 3 THR C 143 VAL C 146 -1 N VAL C 146 O LEU C 114
SHEET 1 J 2 HIS C 107 LEU C 109 0
SHEET 2 J 2 VAL C 175 LEU C 177 1 N VAL C 175 O LEU C 108
SHEET 1 K 4 ASN C 137 GLY C 140 0
SHEET 2 K 4 SER C 127 ARG C 131 -1 N CYS C 130 O ILE C 138
SHEET 3 K 4 GLY C 155 GLN C 163 -1 N LEU C 162 O SER C 127
SHEET 4 K 4 LYS C 166 ILE C 174 -1 N ILE C 174 O GLY C 155
SHEET 1 L 4 LEU L 4 GLN L 6 0
SHEET 2 L 4 ALA L 19 ALA L 25 -1 N ARG L 24 O THR L 5
SHEET 3 L 4 GLU L 70 ILE L 75 -1 N ILE L 75 O ALA L 19
SHEET 4 L 4 PHE L 62 SER L 67 -1 N SER L 67 O GLU L 70
SHEET 1 M 5 THR L 10 VAL L 13 0
SHEET 2 M 5 THR L 104 ILE L 108 1 N ARG L 105 O LEU L 11
SHEET 3 M 5 ALA L 84 GLN L 90 -1 N TYR L 86 O THR L 104
SHEET 4 M 5 LEU L 33 GLN L 38 -1 N GLN L 38 O VAL L 85
SHEET 5 M 5 ARG L 45 ILE L 48 -1 N ILE L 48 O TRP L 35
SHEET 1 N 4 SER L 116 PHE L 120 0
SHEET 2 N 4 THR L 131 ASN L 139 -1 N ASN L 139 O SER L 116
SHEET 3 N 4 LEU L 177 SER L 184 -1 N LEU L 183 O ALA L 132
SHEET 4 N 4 SER L 161 VAL L 165 -1 N SER L 164 O SER L 178
SHEET 1 O 3 LYS L 147 TRP L 150 0
SHEET 2 O 3 VAL L 193 THR L 199 -1 N THR L 199 O LYS L 147
SHEET 3 O 3 VAL L 207 ASN L 212 -1 N PHE L 211 O TYR L 194
SHEET 1 P 4 GLN H 3 GLU H 6 0
SHEET 2 P 4 VAL H 18 SER H 25 -1 N SER H 25 O GLN H 3
SHEET 3 P 4 THR H 78 LEU H 83 -1 N LEU H 83 O VAL H 18
SHEET 4 P 4 VAL H 68 ASP H 73 -1 N ASP H 73 O THR H 78
SHEET 1 Q 6 GLU H 10 LYS H 12 0
SHEET 2 Q 6 THR H 122 VAL H 126 1 N THR H 125 O GLU H 10
SHEET 3 Q 6 ALA H 92 TYR H 100 -1 N TYR H 94 O THR H 122
SHEET 4 Q 6 TYR H 32 GLN H 39 -1 N GLN H 39 O VAL H 93
SHEET 5 Q 6 LEU H 45 ILE H 52 -1 N ILE H 51 O PHE H 34
SHEET 6 Q 6 VAL H 57 TYR H 60 -1 N HIS H 59 O ARG H 50
SHEET 1 R 4 SER H 135 LEU H 139 0
SHEET 2 R 4 THR H 150 TYR H 160 -1 N LYS H 158 O SER H 135
SHEET 3 R 4 TYR H 191 PRO H 200 -1 N VAL H 199 O ALA H 151
SHEET 4 R 4 VAL H 178 THR H 180 -1 N HIS H 179 O VAL H 196
SHEET 1 S 3 VAL H 165 TRP H 169 0
SHEET 2 S 3 ILE H 210 HIS H 215 -1 N ASN H 214 O THR H 166
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FIG. 53-8

```
SSBOND  1 CYS G 119   CYS G 205
SSBOND  2 CYS G 126   CYS G 196
SSBOND  3 CYS G 218   CYS G 247
SSBOND  4 CYS G 228   CYS G 239
SSBOND  5 CYS G 296   CYS G 331
SSBOND  6 CYS G 378   CYS G 445
SSBOND  7 CYS G 385   CYS G 418
SSBOND  8 CYS C  16   CYS C  84
SSBOND  9 CYS C 130   CYS C 159
SSBOND 10 CYS L  23   CYS L  88
SSBOND 11 CYS L 136   CYS L 196
SSBOND 12 CYS H  22   CYS H  96
SSBOND 13 CYS H 155   CYS H 211
LINK        C1  NAG G 697          ND2 ASN G 197
LINK        C1  NAG G 734          ND2 ASN G 234
LINK        O6  NAG G 734          C1  FUC G 735
LINK        C1  NAG G 762          ND2 ASN G 262
LINK        C1  NAG G 776          ND2 ASN G 276
LINK        C1  NAG G 789          ND2 ASN G 289
LINK        C1  NAG G 795          ND2 ASN G 295
LINK        O6  NAG G 795          C1  FUC G 796
LINK        C1  NAG G 832          ND2 ASN G 332
LINK        C1  NAG G 839          ND2 ASN G 339
LINK        C1  NAG G 886          ND2 ASN G 386
LINK        C1  NAG G 892          ND2 ASN G 392
LINK        O6  NAG G 892          C1  FUC G 893
LINK        C1  NAG G 948          ND2 ASN G 448
LINK        O6  NAG G 948          C1  FUC G 949
CISPEP  1 TRP L  94   PRO L  95     0      -1.61
SITE    1   O  1 HOH 1000
CRYST1   71.640   88.130  196.700  90.00  90.00  90.00 P 2 2 21     4
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.013959  0.000000  0.000000        0.00000
SCALE2      0.000000  0.011347  0.000000        0.00000
SCALE3      0.000000  0.000000  0.005084        0.00000
ATOM      1  N   THR G  90      30.031 -50.064  78.936  1.00 42.55           N
ATOM      2  CA  THR G  90      30.956 -49.288  79.751  1.00 43.59           C
ATOM      3  C   THR G  90      32.160 -48.859  78.914  1.00 43.84           C
ATOM      4  O   THR G  90      32.133 -48.983  77.690  1.00 43.64           O
ATOM      5  CB  THR G  90      31.434 -50.091  80.976  1.00 43.87           C
ATOM      6  OG1 THR G  90      32.164 -49.231  81.860  1.00 44.69           O
ATOM      7  CG2 THR G  90      32.341 -51.244  80.546  1.00 44.10           C
ATOM      8  N   GLU G  91      33.197 -48.347  79.579  1.00 44.15           N
ATOM      9  CA  GLU G  91      34.411 -47.885  78.916  1.00 44.60           C
ATOM     10  C   GLU G  91      34.013 -47.006  77.729  1.00 44.76           C
ATOM     11  O   GLU G  91      34.031 -47.437  76.570  1.00 44.30           O
ATOM     12  CB  GLU G  91      35.268 -49.083  78.488  1.00 45.29           C
ATOM     13  CG  GLU G  91      36.609 -48.739  77.835  1.00 46.21           C
ATOM     14  CD  GLU G  91      37.492 -47.838  78.686  1.00 46.69           C
ATOM     15  OE1 GLU G  91      37.408 -47.892  79.934  1.00 46.43           O
ATOM     16  OE2 GLU G  91      38.283 -47.074  78.097  1.00 46.96           O
ATOM     17  N   ASN G  92      33.606 -45.779  78.038  1.00 45.37           N
ATOM     18  CA  ASN G  92      33.158 -44.849  77.011  1.00 45.12           C
ATOM     19  C   ASN G  92      33.960 -43.555  77.009  1.00 43.64           C
ATOM     20  O   ASN G  92      34.841 -43.357  77.844  1.00 43.30           O
ATOM     21  CB  ASN G  92      31.670 -44.551  77.193  1.00 46.34           C
ATOM     22  CG  ASN G  92      30.946 -44.408  75.875  1.00 47.98           C
ATOM     23  OD1 ASN G  92      30.957 -43.340  75.264  1.00 50.80           O
ATOM     24  ND2 ASN G  92      30.327 -45.488  75.414  1.00 46.76           N
ATOM     25  N   PHE G  93      33.643 -42.671  76.072  1.00 42.38           N
ATOM     26  CA  PHE G  93      34.349 -41.405  75.954  1.00 41.75           C
ATOM     27  C   PHE G  93      33.480 -40.164  76.196  1.00 40.40           C
ATOM     28  O   PHE G  93      32.328 -40.096  75.745  1.00 39.86           O
ATOM     29  CB  PHE G  93      35.022 -41.319  74.582  1.00 42.32           C
ATOM     30  CG  PHE G  93      35.668 -39.999  74.316  1.00 44.10           C
ATOM     31  CD1 PHE G  93      36.893 -39.686  74.886  1.00 44.33           C
ATOM     32  CD2 PHE G  93      35.035 -39.055  73.513  1.00 44.30           C
ATOM     33  CE1 PHE G  93      37.480 -38.453  74.663  1.00 44.98           C
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FIG. 53-9

ATOM	35	CZ	PHE	G	93	36.837	-37.516	73.858	1.00	43.72	C
ATOM	36	N	ASN	G	94	34.077	-39.182	76.873	1.00	39.00	N
ATOM	37	CA	ASN	G	94	33.454	-37.897	77.210	1.00	37.42	C
ATOM	38	C	ASN	G	94	34.517	-36.797	77.002	1.00	37.03	C
ATOM	39	O	ASN	G	94	35.710	-37.108	76.896	1.00	36.49	O
ATOM	40	CB	ASN	G	94	33.002	-37.896	78.679	1.00	35.90	C
ATOM	41	CG	ASN	G	94	31.830	-38.834	78.945	1.00	34.52	C
ATOM	42	OD1	ASN	G	94	31.979	-40.057	78.952	1.00	33.54	O
ATOM	43	ND2	ASN	G	94	30.665	-38.261	79.205	1.00	34.56	N
ATOM	44	N	MET	G	95	34.107	-35.524	76.958	1.00	37.83	N
ATOM	45	CA	MET	G	95	35.065	-34.420	76.771	1.00	37.72	C
ATOM	46	C	MET	G	95	34.533	-32.980	76.950	1.00	37.31	C
ATOM	47	O	MET	G	95	33.358	-32.757	77.251	1.00	36.78	O
ATOM	48	CB	MET	G	95	35.718	-34.519	75.389	1.00	38.12	C
ATOM	49	CG	MET	G	95	34.916	-33.849	74.288	1.00	40.14	C
ATOM	50	SD	MET	G	95	35.944	-32.921	73.115	1.00	42.89	S
ATOM	51	CE	MET	G	95	37.369	-32.474	74.135	1.00	40.97	C
ATOM	52	N	TRP	G	96	35.426	-32.017	76.698	1.00	36.64	N
ATOM	53	CA	TRP	G	96	35.167	-30.571	76.769	1.00	34.44	C
ATOM	54	C	TRP	G	96	34.325	-30.111	75.579	1.00	32.91	C
ATOM	55	O	TRP	G	96	34.619	-29.091	74.957	1.00	31.85	O
ATOM	56	CB	TRP	G	96	36.504	-29.803	76.747	1.00	33.83	C
ATOM	57	CG	TRP	G	96	36.980	-29.352	78.091	1.00	33.15	C
ATOM	58	CD1	TRP	G	96	37.581	-30.109	79.045	1.00	33.76	C
ATOM	59	CD2	TRP	G	96	36.830	-28.044	78.652	1.00	34.00	C
ATOM	60	NE1	TRP	G	96	37.806	-29.360	80.175	1.00	35.56	N
ATOM	61	CE2	TRP	G	96	37.352	-28.087	79.960	1.00	34.55	C
ATOM	62	CE3	TRP	G	96	36.296	-26.836	78.177	1.00	32.92	C
ATOM	63	CZ2	TRP	G	96	37.355	-26.971	80.800	1.00	34.75	C
ATOM	64	CZ3	TRP	G	96	36.301	-25.733	79.008	1.00	32.95	C
ATOM	65	CH2	TRP	G	96	36.827	-25.806	80.307	1.00	33.90	C
ATOM	66	N	LYS	G	97	33.284	-30.874	75.270	1.00	33.26	N
ATOM	67	CA	LYS	G	97	32.403	-30.595	74.142	1.00	32.78	C
ATOM	68	C	LYS	G	97	31.005	-30.221	74.632	1.00	32.62	C
ATOM	69	O	LYS	G	97	30.731	-29.041	74.878	1.00	33.71	O
ATOM	70	CB	LYS	G	97	32.382	-31.812	73.189	1.00	32.07	C
ATOM	71	CG	LYS	G	97	31.271	-31.849	72.148	1.00	31.66	C
ATOM	72	CD	LYS	G	97	31.240	-30.621	71.251	1.00	31.98	C
ATOM	73	CE	LYS	G	97	32.430	-30.554	70.323	1.00	31.95	C
ATOM	74	NZ	LYS	G	97	32.231	-29.456	69.345	1.00	32.73	N
ATOM	75	N	ASN	G	98	30.137	-31.212	74.829	1.00	31.57	N
ATOM	76	CA	ASN	G	98	28.792	-30.901	75.276	1.00	32.25	C
ATOM	77	C	ASN	G	98	28.005	-32.017	75.980	1.00	32.40	C
ATOM	78	O	ASN	G	98	28.553	-32.777	76.776	1.00	31.37	O
ATOM	79	CB	ASN	G	98	27.987	-30.305	74.106	1.00	31.45	C
ATOM	80	CG	ASN	G	98	27.745	-31.296	72.972	1.00	31.55	C
ATOM	81	OD1	ASN	G	98	27.136	-30.945	71.961	1.00	30.95	O
ATOM	82	ND2	ASN	G	98	28.201	-32.535	73.137	1.00	31.27	N
ATOM	83	N	ASP	G	99	26.698	-31.999	75.737	1.00	33.77	N
ATOM	84	CA	ASP	G	99	25.677	-32.922	76.237	1.00	34.41	C
ATOM	85	C	ASP	G	99	24.477	-32.005	76.177	1.00	35.14	C
ATOM	86	O	ASP	G	99	23.555	-32.199	75.387	1.00	36.80	O
ATOM	87	CB	ASP	G	99	25.875	-33.361	77.690	1.00	32.72	C
ATOM	88	CG	ASP	G	99	24.658	-34.115	78.232	1.00	31.32	C
ATOM	89	OD1	ASP	G	99	24.205	-35.055	77.553	1.00	32.59	O
ATOM	90	OD2	ASP	G	99	24.127	-33.759	79.307	1.00	28.70	O
ATOM	91	N	MET	G	100	24.583	-30.919	76.929	1.00	35.52	N
ATOM	92	CA	MET	G	100	23.551	-29.907	76.990	1.00	35.08	C
ATOM	93	C	MET	G	100	24.197	-28.533	77.060	1.00	33.39	C
ATOM	94	O	MET	G	100	23.511	-27.557	77.314	1.00	33.51	O
ATOM	95	CB	MET	G	100	22.666	-30.103	78.227	1.00	38.36	C
ATOM	96	CG	MET	G	100	21.768	-31.322	78.195	1.00	40.24	C
ATOM	97	SD	MET	G	100	20.544	-31.193	76.890	1.00	41.93	S
ATOM	98	CE	MET	G	100	20.653	-32.816	76.172	1.00	39.92	C
ATOM	99	N	VAL	G	101	25.511	-28.441	76.860	1.00	31.09	N
ATOM	100	CA	VAL	G	101	26.157	-27.131	76.921	1.00	27.99	C
ATOM	101	C	VAL	G	101	25.490	-26.185	75.910	1.00	26.63	C
ATOM	102	O	VAL	G	101	24.965	-25.138	76.295	1.00	27.19	O
ATOM	103	CB	VAL	G	101	27.684	-27.211	76.701	1.00	26.80	C
ATOM	104	CG1	VAL	G	101	28.314	-25.833	76.875	1.00	23.64	C

FIG. 53-10

ATOM	106	N	GLU	G	102	25.453	-26.572	74.639	1.00	23.53	N
ATOM	107	CA	GLU	G	102	24.805	-25.744	73.629	1.00	21.32	C
ATOM	108	C	GLU	G	102	23.298	-25.708	73.838	1.00	20.85	C
ATOM	109	O	GLU	G	102	22.665	-24.674	73.615	1.00	23.56	O
ATOM	110	CB	GLU	G	102	25.114	-26.253	72.225	1.00	20.82	C
ATOM	111	CG	GLU	G	102	26.375	-25.686	71.605	1.00	18.31	C
ATOM	112	CD	GLU	G	102	27.622	-25.948	72.431	1.00	16.74	C
ATOM	113	OE1	GLU	G	102	27.821	-27.107	72.870	1.00	14.69	O
ATOM	114	OE2	GLU	G	102	28.403	-24.988	72.635	1.00	14.10	O
ATOM	115	N	GLN	G	103	22.726	-26.841	74.250	1.00	18.06	N
ATOM	116	CA	GLN	G	103	21.283	-26.971	74.499	1.00	16.18	C
ATOM	117	C	GLN	G	103	20.860	-26.063	75.645	1.00	14.68	C
ATOM	118	O	GLN	G	103	20.054	-25.155	75.461	1.00	16.26	O
ATOM	119	CB	GLN	G	103	20.933	-28.419	74.859	1.00	17.03	C
ATOM	120	CG	GLN	G	103	19.845	-29.041	74.004	1.00	16.72	C
ATOM	121	CD	GLN	G	103	18.527	-28.346	74.159	1.00	17.00	C
ATOM	122	OE1	GLN	G	103	18.001	-27.767	73.209	1.00	16.51	O
ATOM	123	NE2	GLN	G	103	17.961	-28.425	75.352	1.00	19.08	N
ATOM	124	N	MET	G	104	21.383	-26.352	76.832	1.00	11.83	N
ATOM	125	CA	MET	G	104	21.128	-25.583	78.043	1.00	11.35	C
ATOM	126	C	MET	G	104	21.302	-24.091	77.761	1.00	11.72	C
ATOM	127	O	MET	G	104	20.382	-23.305	77.997	1.00	10.83	O
ATOM	128	CB	MET	G	104	22.121	-26.001	79.120	1.00	11.71	C
ATOM	129	CG	MET	G	104	21.764	-25.618	80.530	1.00	11.54	C
ATOM	130	SD	MET	G	104	23.083	-26.186	81.587	1.00	11.76	S
ATOM	131	CE	MET	G	104	22.640	-25.382	83.126	1.00	13.15	C
ATOM	132	N	HIS	G	105	22.463	-23.711	77.220	1.00	11.06	N
ATOM	133	CA	HIS	G	105	22.746	-22.314	76.893	1.00	11.77	C
ATOM	134	C	HIS	G	105	21.541	-21.681	76.196	1.00	13.11	C
ATOM	135	O	HIS	G	105	21.053	-20.637	76.625	1.00	12.48	O
ATOM	136	CB	HIS	G	105	23.995	-22.199	76.008	1.00	10.23	C
ATOM	137	CG	HIS	G	105	24.614	-20.839	76.003	1.00	8.87	C
ATOM	138	ND1	HIS	G	105	24.918	-20.177	77.167	1.00	7.75	N
ATOM	139	CD2	HIS	G	105	25.039	-20.085	74.950	1.00	10.05	C
ATOM	140	CE1	HIS	G	105	25.513	-19.058	76.810	1.00	9.56	C
ATOM	141	NE2	HIS	G	105	25.611	-18.954	75.475	1.00	7.33	N
ATOM	142	N	GLU	G	106	20.998	-22.370	75.194	1.00	15.32	N
ATOM	143	CA	GLU	G	106	19.843	-21.862	74.469	1.00	17.17	C
ATOM	144	C	GLU	G	106	18.564	-21.908	75.293	1.00	17.51	C
ATOM	145	O	GLU	G	106	17.652	-21.115	75.060	1.00	19.56	O
ATOM	146	CB	GLU	G	106	19.663	-22.586	73.132	1.00	20.59	C
ATOM	147	CG	GLU	G	106	20.773	-22.299	72.104	1.00	28.21	C
ATOM	148	CD	GLU	G	106	20.999	-20.802	71.832	1.00	32.28	C
ATOM	149	OE1	GLU	G	106	20.005	-20.050	71.719	1.00	34.24	O
ATOM	150	OE2	GLU	G	106	22.179	-20.386	71.723	1.00	31.84	O
ATOM	151	N	ASP	G	107	18.477	-22.823	76.254	1.00	17.54	N
ATOM	152	CA	ASP	G	107	17.283	-22.881	77.101	1.00	17.03	C
ATOM	153	C	ASP	G	107	17.315	-21.697	78.059	1.00	14.26	C
ATOM	154	O	ASP	G	107	16.332	-20.973	78.207	1.00	11.84	O
ATOM	155	CB	ASP	G	107	17.225	-24.182	77.899	1.00	21.39	C
ATOM	156	CG	ASP	G	107	16.535	-25.310	77.140	1.00	26.46	C
ATOM	157	OD1	ASP	G	107	15.279	-25.348	77.098	1.00	28.30	O
ATOM	158	OD2	ASP	G	107	17.254	-26.195	76.628	1.00	28.96	O
ATOM	159	N	ILE	G	108	18.478	-21.486	78.674	1.00	13.84	N
ATOM	160	CA	ILE	G	108	18.711	-20.388	79.615	1.00	12.27	C
ATOM	161	C	ILE	G	108	18.596	-19.027	78.928	1.00	12.24	C
ATOM	162	O	ILE	G	108	17.996	-18.103	79.477	1.00	14.39	O
ATOM	163	CB	ILE	G	108	20.074	-20.519	80.303	1.00	10.08	C
ATOM	164	CG1	ILE	G	108	20.227	-21.943	80.871	1.00	9.55	C
ATOM	165	CG2	ILE	G	108	20.191	-19.495	81.422	1.00	8.16	C
ATOM	166	CD1	ILE	G	108	19.022	-22.441	81.680	1.00	2.00	C
ATOM	167	N	ILE	G	109	19.139	-18.897	77.723	1.00	9.86	N
ATOM	168	CA	ILE	G	109	19.004	-17.640	77.006	1.00	8.89	C
ATOM	169	C	ILE	G	109	17.518	-17.407	76.764	1.00	7.93	C
ATOM	170	O	ILE	G	109	17.022	-16.303	76.938	1.00	9.04	O
ATOM	171	CB	ILE	G	109	19.745	-17.633	75.642	1.00	7.59	C
ATOM	172	CG1	ILE	G	109	21.255	-17.655	75.854	1.00	5.11	C
ATOM	173	CG2	ILE	G	109	19.413	-16.368	74.874	1.00	9.22	C
ATOM	174	CD1	ILE	G	109	22.033	-17.460	74.588	1.00	3.72	C
ATOM	175	N	SER	G	110	16.791	-18.463	76.436	1.00	7.89	N

FIG. 53-11

ATOM	177	C	SER	G	110	14.530	-18.251	77.454	1.00	11.75	C
ATOM	178	O	SER	G	110	13.324	-17.967	77.425	1.00	11.41	O
ATOM	179	CB	SER	G	110	14.886	-19.477	75.283	1.00	9.57	C
ATOM	180	OG	SER	G	110	15.657	-19.524	74.088	1.00	8.93	O
ATOM	181	N	LEU	G	111	15.174	-18.511	78.584	1.00	13.81	N
ATOM	182	CA	LEU	G	111	14.495	-18.467	79.867	1.00	14.15	C
ATOM	183	C	LEU	G	111	14.586	-17.035	80.380	1.00	15.33	C
ATOM	184	O	LEU	G	111	13.588	-16.428	80.786	1.00	14.92	O
ATOM	185	CB	LEU	G	111	15.159	-19.445	80.831	1.00	13.12	C
ATOM	186	CG	LEU	G	111	14.248	-19.938	81.949	1.00	14.99	C
ATOM	187	CD1	LEU	G	111	14.601	-21.370	82.306	1.00	16.86	C
ATOM	188	CD2	LEU	G	111	14.349	-19.008	83.150	1.00	14.95	C
ATOM	189	N	TRP	G	112	15.785	-16.476	80.286	1.00	16.51	N
ATOM	190	CA	TRP	G	112	16.031	-15.113	80.715	1.00	17.45	C
ATOM	191	C	TRP	G	112	15.124	-14.162	79.974	1.00	18.63	C
ATOM	192	O	TRP	G	112	14.487	-13.314	80.592	1.00	21.62	O
ATOM	193	CB	TRP	G	112	17.481	-14.741	80.465	1.00	16.89	C
ATOM	194	CG	TRP	G	112	18.347	-15.026	81.623	1.00	15.36	C
ATOM	195	CD1	TRP	G	112	18.492	-16.216	82.278	1.00	13.64	C
ATOM	196	CD2	TRP	G	112	19.175	-14.086	82.302	1.00	14.57	C
ATOM	197	NE1	TRP	G	112	19.360	-16.068	83.331	1.00	14.50	N
ATOM	198	CE2	TRP	G	112	19.793	-14.769	83.369	1.00	14.49	C
ATOM	199	CE3	TRP	G	112	19.453	-12.728	82.113	1.00	11.21	C
ATOM	200	CZ2	TRP	G	112	20.675	-14.137	84.245	1.00	13.94	C
ATOM	201	CZ3	TRP	G	112	20.324	-12.103	82.979	1.00	11.75	C
ATOM	202	CH2	TRP	G	112	20.926	-12.804	84.033	1.00	13.78	C
ATOM	203	N	ASP	G	113	15.051	-14.323	78.658	1.00	18.33	N
ATOM	204	CA	ASP	G	113	14.208	-13.490	77.818	1.00	19.69	C
ATOM	205	C	ASP	G	113	12.776	-13.400	78.354	1.00	21.06	C
ATOM	206	O	ASP	G	113	12.250	-12.302	78.544	1.00	21.21	O
ATOM	207	CB	ASP	G	113	14.200	-14.022	76.377	1.00	19.57	C
ATOM	208	CG	ASP	G	113	15.518	-13.767	75.633	1.00	19.88	C
ATOM	209	OD1	ASP	G	113	16.541	-13.418	76.267	1.00	18.64	O
ATOM	210	OD2	ASP	G	113	15.527	-13.928	74.391	1.00	19.87	O
ATOM	211	N	GLN	G	114	12.156	-14.553	78.618	1.00	23.29	N
ATOM	212	CA	GLN	G	114	10.776	-14.604	79.131	1.00	24.16	C
ATOM	213	C	GLN	G	114	10.638	-14.027	80.545	1.00	24.98	C
ATOM	214	O	GLN	G	114	9.553	-13.601	80.946	1.00	25.23	O
ATOM	215	CB	GLN	G	114	10.228	-16.048	79.117	1.00	23.58	C
ATOM	216	CG	GLN	G	114	10.735	-16.953	80.263	1.00	23.77	C
ATOM	217	CD	GLN	G	114	10.087	-18.346	80.303	1.00	21.80	C
ATOM	218	OE1	GLN	G	114	9.657	-18.810	81.357	1.00	20.50	O
ATOM	219	NE2	GLN	G	114	10.071	-19.030	79.172	1.00	20.83	N
ATOM	220	N	SER	G	115	11.739	-13.989	81.286	1.00	26.32	N
ATOM	221	CA	SER	G	115	11.724	-13.482	82.649	1.00	28.15	C
ATOM	222	C	SER	G	115	12.191	-12.033	82.789	1.00	27.92	C
ATOM	223	O	SER	G	115	11.367	-11.109	82.795	1.00	29.96	O
ATOM	224	CB	SER	G	115	12.549	-14.409	83.547	1.00	31.07	C
ATOM	225	OG	SER	G	115	12.333	-14.132	84.920	1.00	35.36	O
ATOM	226	N	LEU	G	116	13.506	-11.829	82.870	1.00	26.47	N
ATOM	227	CA	LEU	G	116	14.096	-10.494	83.041	1.00	24.17	C
ATOM	228	C	LEU	G	116	14.051	-9.630	81.788	1.00	23.78	C
ATOM	229	O	LEU	G	116	15.038	-9.517	81.068	1.00	24.42	O
ATOM	230	CB	LEU	G	116	15.546	-10.616	83.522	1.00	22.24	C
ATOM	231	CG	LEU	G	116	15.833	-11.024	84.969	1.00	19.18	C
ATOM	232	CD1	LEU	G	116	17.241	-11.555	85.085	1.00	17.42	C
ATOM	233	CD2	LEU	G	116	15.634	-9.831	85.893	1.00	20.14	C
ATOM	234	N	LYS	G	117	12.902	-9.017	81.536	1.00	24.32	N
ATOM	235	CA	LYS	G	117	12.727	-8.150	80.372	1.00	24.12	C
ATOM	236	C	LYS	G	117	13.301	-6.739	80.575	1.00	24.20	C
ATOM	237	O	LYS	G	117	13.048	-6.083	81.591	1.00	22.60	O
ATOM	238	CB	LYS	G	117	11.248	-8.078	79.975	1.00	23.53	C
ATOM	239	CG	LYS	G	117	10.791	-9.215	79.061	1.00	24.11	C
ATOM	240	CD	LYS	G	117	9.275	-9.287	78.933	1.00	22.89	C
ATOM	241	CE	LYS	G	117	8.693	-10.447	79.750	1.00	22.26	C
ATOM	242	NZ	LYS	G	117	8.938	-10.378	81.232	1.00	21.42	N
ATOM	243	N	PRO	G	118	14.136	-6.282	79.630	1.00	24.87	N
ATOM	244	CA	PRO	G	118	14.745	-4.957	79.708	1.00	26.24	C
ATOM	245	C	PRO	G	118	14.215	-4.016	78.632	1.00	28.46	C
ATOM	246	O	PRO	G	118	13.010	-3.918	78.371	1.00	27.89	O

FIG. 53-12

ATOM	248	CG	PRO	G	118	16.058	-6.227	78.276	1.00	24.79	C
ATOM	249	CD	PRO	G	118	14.907	-7.134	78.705	1.00	25.85	C
ATOM	250	N	CYS	G	119	15.166	-3.317	78.023	1.00	30.90	N
ATOM	251	CA	CYS	G	119	14.951	-2.361	76.955	1.00	32.05	C
ATOM	252	C	CYS	G	119	16.293	-2.538	76.185	1.00	30.56	C
ATOM	253	O	CYS	G	119	17.284	-1.848	76.424	1.00	30.87	O
ATOM	254	CB	CYS	G	119	14.726	-0.972	77.587	1.00	33.32	C
ATOM	255	SG	CYS	G	119	13.194	-0.851	78.612	1.00	39.28	S
ATOM	256	N	VAL	G	120	16.312	-3.605	75.382	1.00	29.90	N
ATOM	257	CA	VAL	G	120	17.451	-4.101	74.585	1.00	27.91	C
ATOM	258	C	VAL	G	120	18.028	-3.209	73.489	1.00	27.39	C
ATOM	259	O	VAL	G	120	17.368	-2.310	73.002	1.00	29.19	O
ATOM	260	CB	VAL	G	120	17.082	-5.472	73.916	1.00	26.78	C
ATOM	261	CG1	VAL	G	120	18.324	-6.242	73.535	1.00	26.16	C
ATOM	262	CG2	VAL	G	120	16.206	-6.312	74.826	1.00	25.20	C
ATOM	263	N	LYS	G	121	19.251	-3.515	73.073	1.00	27.48	N
ATOM	264	CA	LYS	G	121	19.934	-2.790	72.011	1.00	28.16	C
ATOM	265	C	LYS	G	121	21.093	-3.658	71.491	1.00	28.51	C
ATOM	266	O	LYS	G	121	22.133	-3.779	72.143	1.00	27.76	O
ATOM	267	CB	LYS	G	121	20.450	-1.448	72.536	1.00	28.76	C
ATOM	268	CG	LYS	G	121	20.477	-0.360	71.480	1.00	28.67	C
ATOM	269	CD	LYS	G	121	20.967	0.952	72.030	1.00	29.16	C
ATOM	270	CE	LYS	G	121	22.438	0.889	72.369	1.00	29.64	C
ATOM	271	NZ	LYS	G	121	23.025	2.251	72.244	1.00	32.93	N
ATOM	272	N	LEU	G	122	20.890	-4.280	70.332	1.00	29.13	N
ATOM	273	CA	LEU	G	122	21.882	-5.169	69.721	1.00	29.85	C
ATOM	274	C	LEU	G	122	22.306	-4.696	68.330	1.00	31.68	C
ATOM	275	O	LEU	G	122	21.480	-4.206	67.557	1.00	30.70	O
ATOM	276	CB	LEU	G	122	21.333	-6.598	69.631	1.00	29.20	C
ATOM	277	CG	LEU	G	122	19.973	-6.806	68.952	1.00	29.73	C
ATOM	278	CD1	LEU	G	122	19.854	-8.232	68.431	1.00	29.60	C
ATOM	279	CD2	LEU	G	122	18.832	-6.471	69.903	1.00	28.04	C
ATOM	280	N	THR	G	123	23.573	-4.922	67.988	1.00	35.02	N
ATOM	281	CA	THR	G	123	24.128	-4.486	66.708	1.00	39.27	C
ATOM	282	C	THR	G	123	24.276	-5.430	65.517	1.00	43.14	C
ATOM	283	O	THR	G	123	25.073	-6.368	65.563	1.00	45.11	O
ATOM	284	CB	THR	G	123	25.533	-3.877	66.890	1.00	39.33	C
ATOM	285	OG1	THR	G	123	26.257	-4.621	67.883	1.00	37.86	O
ATOM	286	CG2	THR	G	123	25.451	-2.402	67.271	1.00	40.77	C
ATOM	287	N	PRO	G	124	23.466	-5.240	64.468	1.00	45.88	N
ATOM	288	CA	PRO	G	124	23.513	-6.047	63.242	1.00	47.10	C
ATOM	289	C	PRO	G	124	24.355	-5.185	62.292	1.00	47.86	C
ATOM	290	O	PRO	G	124	24.015	-4.029	62.048	1.00	46.46	O
ATOM	291	CB	PRO	G	124	22.051	-6.114	62.814	1.00	47.28	C
ATOM	292	CG	PRO	G	124	21.510	-4.836	63.265	1.00	47.43	C
ATOM	293	CD	PRO	G	124	22.137	-4.620	64.617	1.00	46.92	C
ATOM	294	N	LEU	G	125	25.461	-5.713	61.786	1.00	50.15	N
ATOM	295	CA	LEU	G	125	26.324	-4.890	60.946	1.00	53.58	C
ATOM	296	C	LEU	G	125	26.012	-4.529	59.498	1.00	55.92	C
ATOM	297	O	LEU	G	125	25.466	-5.314	58.719	1.00	55.97	O
ATOM	298	CB	LEU	G	125	27.797	-5.259	61.136	1.00	53.97	C
ATOM	299	CG	LEU	G	125	28.463	-4.311	62.143	1.00	54.12	C
ATOM	300	CD1	LEU	G	125	28.818	-2.975	61.498	1.00	54.49	C
ATOM	301	CD2	LEU	G	125	27.536	-4.081	63.328	1.00	54.73	C
ATOM	302	N	CYS	G	126	26.422	-3.305	59.178	1.00	58.50	N
ATOM	303	CA	CYS	G	126	26.244	-2.634	57.896	1.00	60.18	C
ATOM	304	C	CYS	G	126	26.585	-3.269	56.557	1.00	59.83	C
ATOM	305	O	CYS	G	126	27.185	-4.339	56.458	1.00	59.92	O
ATOM	306	CB	CYS	G	126	26.951	-1.283	57.945	1.00	61.77	C
ATOM	307	SG	CYS	G	126	26.277	-0.089	59.134	1.00	67.19	S
ATOM	308	N	VAL	G	127	26.206	-2.517	55.529	1.00	58.73	N
ATOM	309	CA	VAL	G	127	26.432	-2.814	54.121	1.00	58.05	C
ATOM	310	C	VAL	G	127	26.789	-1.430	53.582	1.00	57.40	C
ATOM	311	O	VAL	G	127	27.888	-1.211	53.066	1.00	57.78	O
ATOM	312	CB	VAL	G	127	25.145	-3.310	53.416	1.00	58.63	C
ATOM	313	CG1	VAL	G	127	25.332	-3.307	51.906	1.00	58.31	C
ATOM	314	CG2	VAL	G	127	24.796	-4.709	53.886	1.00	59.78	C
ATOM	315	N	GLY	G	128	25.869	-0.485	53.773	1.00	56.22	N
ATOM	316	CA	GLY	G	128	26.095	0.879	53.330	1.00	54.59	C
ATOM	317	C	GLY	G	128	24.880	1.554	52.717	1.00	53.61	C

FIG. 53-13

ATOM	319	N	ALA	G	129	25.136	2.639	51.991	1.00	53.86	N
ATOM	320	CA	ALA	G	129	24.107	3.419	51.295	1.00	53.81	C
ATOM	321	C	ALA	G	129	22.957	3.928	52.169	1.00	53.84	C
ATOM	322	O	ALA	G	129	21.794	3.882	51.771	1.00	53.00	O
ATOM	323	CB	ALA	G	129	23.564	2.630	50.092	1.00	53.14	C
ATOM	324	N	GLY	G	194	23.291	4.435	53.351	1.00	54.62	N
ATOM	325	CA	GLY	G	194	22.276	4.956	54.251	1.00	55.99	C
ATOM	326	C	GLY	G	194	21.534	3.878	55.019	1.00	57.37	C
ATOM	327	O	GLY	G	194	20.858	4.169	56.013	1.00	57.33	O
ATOM	328	N	SER	G	195	21.665	2.634	54.566	1.00	58.65	N
ATOM	329	CA	SER	G	195	21.018	1.492	55.195	1.00	59.28	C
ATOM	330	C	SER	G	195	21.997	0.855	56.181	1.00	59.27	C
ATOM	331	O	SER	G	195	23.039	0.321	55.791	1.00	58.61	O
ATOM	332	CB	SER	G	195	20.605	0.477	54.122	1.00	59.90	C
ATOM	333	OG	SER	G	195	19.683	-0.475	54.626	1.00	61.03	O
ATOM	334	N	CYS	G	196	21.662	0.936	57.463	1.00	59.98	N
ATOM	335	CA	CYS	G	196	22.490	0.377	58.527	1.00	60.78	C
ATOM	336	C	CYS	G	196	21.642	0.079	59.756	1.00	59.75	C
ATOM	337	O	CYS	G	196	21.122	0.990	60.400	1.00	60.30	O
ATOM	338	CB	CYS	G	196	23.612	1.348	58.906	1.00	62.88	C
ATOM	339	SG	CYS	G	196	25.173	1.175	57.983	1.00	66.93	S
ATOM	340	N	ASN	G	197	21.472	-1.200	60.059	1.00	57.89	N
ATOM	341	CA	ASN	G	197	20.680	-1.593	61.212	1.00	55.54	C
ATOM	342	C	ASN	G	197	21.464	-1.640	62.523	1.00	52.35	C
ATOM	343	O	ASN	G	197	22.690	-1.738	62.534	1.00	51.55	O
ATOM	344	CB	ASN	G	197	19.912	-2.921	60.968	1.00	58.11	C
ATOM	345	CG	ASN	G	197	20.757	-4.005	60.276	1.00	59.71	C
ATOM	346	OD1	ASN	G	197	21.810	-3.721	59.710	1.00	62.77	O
ATOM	347	ND2	ASN	G	197	20.263	-5.243	60.269	1.00	60.06	N
ATOM	348	N	THR	G	198	20.724	-1.454	63.609	1.00	48.87	N
ATOM	349	CA	THR	G	198	21.197	-1.495	64.995	1.00	44.56	C
ATOM	350	C	THR	G	198	19.882	-1.452	65.755	1.00	41.54	C
ATOM	351	O	THR	G	198	19.346	-0.384	66.035	1.00	42.10	O
ATOM	352	CB	THR	G	198	22.085	-0.293	65.393	1.00	43.77	C
ATOM	353	OG1	THR	G	198	23.364	-0.405	64.755	1.00	43.48	O
ATOM	354	CG2	THR	G	198	22.302	-0.283	66.909	1.00	42.07	C
ATOM	355	N	SER	G	199	19.327	-2.632	65.986	1.00	37.87	N
ATOM	356	CA	SER	G	199	18.039	-2.778	66.642	1.00	35.19	C
ATOM	357	C	SER	G	199	17.930	-2.385	68.103	1.00	32.73	C
ATOM	358	O	SER	G	199	18.608	-2.957	68.963	1.00	32.29	O
ATOM	359	CB	SER	G	199	17.544	-4.213	66.472	1.00	36.29	C
ATOM	360	OG	SER	G	199	18.538	-5.150	66.853	1.00	37.38	O
ATOM	361	N	VAL	G	200	17.065	-1.409	68.374	1.00	29.80	N
ATOM	362	CA	VAL	G	200	16.804	-0.964	69.740	1.00	26.54	C
ATOM	363	C	VAL	G	200	15.398	-1.463	70.022	1.00	24.38	C
ATOM	364	O	VAL	G	200	14.560	-1.492	69.119	1.00	24.85	O
ATOM	365	CB	VAL	G	200	16.850	0.583	69.897	1.00	25.48	C
ATOM	366	CG1	VAL	G	200	18.070	1.152	69.184	1.00	24.83	C
ATOM	367	CG2	VAL	G	200	15.574	1.221	69.389	1.00	25.79	C
ATOM	368	N	ILE	G	201	15.156	-1.927	71.238	1.00	22.71	N
ATOM	369	CA	ILE	G	201	13.832	-2.423	71.601	1.00	21.84	C
ATOM	370	C	ILE	G	201	13.424	-1.849	72.944	1.00	21.54	C
ATOM	371	O	ILE	G	201	14.127	-1.993	73.942	1.00	21.04	O
ATOM	372	CB	ILE	G	201	13.757	-3.973	71.635	1.00	20.77	C
ATOM	373	CG1	ILE	G	201	13.888	-4.537	70.215	1.00	20.78	C
ATOM	374	CG2	ILE	G	201	12.436	-4.419	72.236	1.00	20.16	C
ATOM	375	CD1	ILE	G	201	13.760	-6.045	70.129	1.00	23.33	C
ATOM	376	N	THR	G	202	12.283	-1.179	72.941	1.00	21.75	N
ATOM	377	CA	THR	G	202	11.742	-0.550	74.125	1.00	22.67	C
ATOM	378	C	THR	G	202	10.596	-1.391	74.662	1.00	24.65	C
ATOM	379	O	THR	G	202	9.459	-1.285	74.205	1.00	25.31	O
ATOM	380	CB	THR	G	202	11.241	0.872	73.791	1.00	21.11	C
ATOM	381	OG1	THR	G	202	12.295	1.609	73.158	1.00	20.05	O
ATOM	382	CG2	THR	G	202	10.803	1.602	75.053	1.00	19.42	C
ATOM	383	N	GLN	G	203	10.909	-2.278	75.591	1.00	27.54	N
ATOM	384	CA	GLN	G	203	9.888	-3.133	76.180	1.00	30.82	C
ATOM	385	C	GLN	G	203	9.499	-2.468	77.471	1.00	33.16	C
ATOM	386	O	GLN	G	203	10.235	-1.623	77.986	1.00	32.53	O
ATOM	387	CB	GLN	G	203	10.448	-4.509	76.539	1.00	31.40	C
ATOM	388	CG	GLN	G	203	11.102	-5.279	75.427	1.00	32.25	C

FIG. 53-14

ATOM	390	OE1	GLN	G	203	12.826	-6.912	75.187	1.00	35.60	O
ATOM	391	NE2	GLN	G	203	12.212	-6.383	77.270	1.00	32.67	N
ATOM	392	N	ALA	G	204	8.351	-2.866	78.007	1.00	36.76	N
ATOM	393	CA	ALA	G	204	7.892	-2.330	79.273	1.00	40.59	C
ATOM	394	C	ALA	G	204	8.815	-2.971	80.301	1.00	42.64	C
ATOM	395	O	ALA	G	204	8.514	-4.047	80.819	1.00	43.43	O
ATOM	396	CB	ALA	G	204	6.447	-2.728	79.527	1.00	40.97	C
ATOM	397	N	CYS	G	205	9.999	-2.378	80.451	1.00	44.24	N
ATOM	398	CA	CYS	G	205	11.030	-2.820	81.385	1.00	44.23	C
ATOM	399	C	CYS	G	205	10.325	-3.002	82.743	1.00	44.07	C
ATOM	400	O	CYS	G	205	9.854	-2.030	83.328	1.00	45.34	O
ATOM	401	CB	CYS	G	205	12.133	-1.732	81.451	1.00	43.58	C
ATOM	402	SG	CYS	G	205	13.597	-1.867	80.335	1.00	46.40	S
ATOM	403	N	PRO	G	206	10.144	-4.260	83.202	1.00	43.68	N
ATOM	404	CA	PRO	G	206	9.472	-4.532	84.480	1.00	42.68	C
ATOM	405	C	PRO	G	206	10.306	-5.049	85.652	1.00	41.36	C
ATOM	406	O	PRO	G	206	11.231	-5.851	85.477	1.00	40.87	O
ATOM	407	CB	PRO	G	206	8.440	-5.567	84.079	1.00	43.26	C
ATOM	408	CG	PRO	G	206	9.210	-6.423	83.081	1.00	44.31	C
ATOM	409	CD	PRO	G	206	10.229	-5.495	82.401	1.00	44.01	C
ATOM	410	N	LYS	G	207	9.914	-4.643	86.860	1.00	40.18	N
ATOM	411	CA	LYS	G	207	10.598	-5.057	88.083	1.00	39.24	C
ATOM	412	C	LYS	G	207	10.112	-6.419	88.558	1.00	40.55	C
ATOM	413	O	LYS	G	207	9.253	-6.513	89.436	1.00	41.20	O
ATOM	414	CB	LYS	G	207	10.412	-4.028	89.213	1.00	35.60	C
ATOM	415	CG	LYS	G	207	11.073	-2.676	88.978	1.00	28.24	C
ATOM	416	CD	LYS	G	207	12.523	-2.811	88.527	1.00	20.45	C
ATOM	417	CE	LYS	G	207	13.447	-3.269	89.619	1.00	14.36	C
ATOM	418	NZ	LYS	G	207	14.818	-3.500	89.066	1.00	12.04	N
ATOM	419	N	VAL	G	208	10.652	-7.471	87.958	1.00	40.92	N
ATOM	420	CA	VAL	G	208	10.283	-8.825	88.326	1.00	41.10	C
ATOM	421	C	VAL	G	208	11.416	-9.383	89.178	1.00	42.22	C
ATOM	422	O	VAL	G	208	12.452	-8.733	89.345	1.00	41.88	O
ATOM	423	CB	VAL	G	208	10.086	-9.703	87.064	1.00	40.88	C
ATOM	424	CG1	VAL	G	208	11.435	-10.083	86.454	1.00	40.92	C
ATOM	425	CG2	VAL	G	208	9.255	-10.936	87.392	1.00	40.95	C
ATOM	426	N	SER	G	209	11.211	-10.583	89.708	1.00	42.81	N
ATOM	427	CA	SER	G	209	12.193	-11.271	90.534	1.00	42.90	C
ATOM	428	C	SER	G	209	12.614	-12.559	89.826	1.00	43.05	C
ATOM	429	O	SER	G	209	11.790	-13.447	89.576	1.00	43.93	O
ATOM	430	CB	SER	G	209	11.560	-11.593	91.887	1.00	44.08	C
ATOM	431	OG	SER	G	209	10.172	-11.851	91.723	1.00	44.85	O
ATOM	432	N	PHE	G	210	13.887	-12.645	89.464	1.00	42.58	N
ATOM	433	CA	PHE	G	210	14.395	-13.825	88.774	1.00	41.96	C
ATOM	434	C	PHE	G	210	14.800	-14.899	89.784	1.00	41.92	C
ATOM	435	O	PHE	G	210	15.612	-14.645	90.669	1.00	42.16	O
ATOM	436	CB	PHE	G	210	15.582	-13.440	87.887	1.00	40.06	C
ATOM	437	CG	PHE	G	210	16.117	-14.572	87.061	1.00	39.61	C
ATOM	438	CD1	PHE	G	210	15.277	-15.299	86.225	1.00	39.31	C
ATOM	439	CD2	PHE	G	210	17.460	-14.923	87.131	1.00	39.15	C
ATOM	440	CE1	PHE	G	210	15.765	-16.356	85.466	1.00	38.42	C
ATOM	441	CE2	PHE	G	210	17.960	-15.985	86.369	1.00	39.64	C
ATOM	442	CZ	PHE	G	210	17.108	-16.704	85.540	1.00	38.39	C
ATOM	443	N	GLU	G	211	14.201	-16.084	89.685	1.00	41.43	N
ATOM	444	CA	GLU	G	211	14.537	-17.169	90.601	1.00	40.62	C
ATOM	445	C	GLU	G	211	14.945	-18.405	89.815	1.00	39.25	C
ATOM	446	O	GLU	G	211	14.389	-18.686	88.752	1.00	39.17	O
ATOM	447	CB	GLU	G	211	13.377	-17.492	91.560	1.00	42.31	C
ATOM	448	CG	GLU	G	211	12.269	-18.363	90.988	1.00	44.19	C
ATOM	449	CD	GLU	G	211	11.492	-19.098	92.070	1.00	45.89	C
ATOM	450	OE1	GLU	G	211	12.108	-19.884	92.828	1.00	45.92	O
ATOM	451	OE2	GLU	G	211	10.261	-18.904	92.162	1.00	47.68	O
ATOM	452	N	PRO	G	212	15.985	-19.110	90.284	1.00	38.52	N
ATOM	453	CA	PRO	G	212	16.486	-20.322	89.626	1.00	36.21	C
ATOM	454	C	PRO	G	212	15.734	-21.602	89.983	1.00	33.09	C
ATOM	455	O	PRO	G	212	15.585	-21.959	91.154	1.00	32.86	O
ATOM	456	CB	PRO	G	212	17.945	-20.369	90.077	1.00	37.50	C
ATOM	457	CG	PRO	G	212	17.859	-19.845	91.481	1.00	38.90	C
ATOM	458	CD	PRO	G	212	16.908	-18.665	91.347	1.00	38.66	C
ATOM	459	N	ILE	G	213	15.222	-22.267	88.958	1.00	29.77	N

FIG. 53-15

ATOM	461	C	ILE	G	213	15.478	-24.612	88.691	1.00	24.26	C
ATOM	462	O	ILE	G	213	16.002	-24.562	87.576	1.00	25.13	O
ATOM	463	CB	ILE	G	213	13.235	-23.584	88.230	1.00	23.85	C
ATOM	464	CG1	ILE	G	213	12.002	-23.217	89.051	1.00	22.29	C
ATOM	465	CG2	ILE	G	213	13.020	-24.976	87.659	1.00	23.98	C
ATOM	466	CD1	ILE	G	213	11.675	-24.235	90.116	1.00	19.78	C
ATOM	467	N	PRO	G	214	15.785	-25.570	89.582	1.00	21.57	N
ATOM	468	CA	PRO	G	214	16.711	-26.636	89.203	1.00	19.74	C
ATOM	469	C	PRO	G	214	16.190	-27.279	87.923	1.00	19.30	C
ATOM	470	O	PRO	G	214	15.031	-27.701	87.850	1.00	19.65	O
ATOM	471	CB	PRO	G	214	16.616	-27.596	90.382	1.00	18.78	C
ATOM	472	CG	PRO	G	214	16.379	-26.697	91.512	1.00	20.57	C
ATOM	473	CD	PRO	G	214	15.341	-25.738	90.972	1.00	20.63	C
ATOM	474	N	ILE	G	215	17.011	-27.276	86.888	1.00	18.27	N
ATOM	475	CA	ILE	G	215	16.599	-27.855	85.633	1.00	19.05	C
ATOM	476	C	ILE	G	215	17.188	-29.253	85.428	1.00	21.00	C
ATOM	477	O	ILE	G	215	18.392	-29.474	85.572	1.00	21.46	O
ATOM	478	CB	ILE	G	215	16.939	-26.922	84.450	1.00	18.63	C
ATOM	479	CG1	ILE	G	215	18.449	-26.688	84.350	1.00	18.94	C
ATOM	480	CG2	ILE	G	215	16.207	-25.594	84.611	1.00	17.22	C
ATOM	481	CD1	ILE	G	215	18.865	-25.836	83.153	1.00	18.67	C
ATOM	482	N	HIS	G	216	16.314	-30.214	85.169	1.00	21.88	N
ATOM	483	CA	HIS	G	216	16.747	-31.572	84.933	1.00	22.93	C
ATOM	484	C	HIS	G	216	16.771	-31.766	83.424	1.00	23.43	C
ATOM	485	O	HIS	G	216	15.853	-31.323	82.734	1.00	23.56	O
ATOM	486	CB	HIS	G	216	15.762	-32.561	85.556	1.00	24.82	C
ATOM	487	CG	HIS	G	216	15.771	-32.576	87.052	1.00	28.60	C
ATOM	488	ND1	HIS	G	216	16.921	-32.414	87.793	1.00	31.33	N
ATOM	489	CD2	HIS	G	216	14.770	-32.751	87.945	1.00	30.95	C
ATOM	490	CE1	HIS	G	216	16.629	-32.492	89.080	1.00	32.29	C
ATOM	491	NE2	HIS	G	216	15.328	-32.696	89.200	1.00	32.75	N
ATOM	492	N	TYR	G	217	17.860	-32.320	82.901	1.00	22.34	N
ATOM	493	CA	TYR	G	217	17.939	-32.596	81.473	1.00	22.17	C
ATOM	494	C	TYR	G	217	17.934	-34.095	81.269	1.00	23.92	C
ATOM	495	O	TYR	G	217	18.844	-34.806	81.719	1.00	24.28	O
ATOM	496	CB	TYR	G	217	19.164	-31.957	80.839	1.00	20.79	C
ATOM	497	CG	TYR	G	217	18.885	-30.558	80.372	1.00	22.08	C
ATOM	498	CD1	TYR	G	217	17.960	-30.322	79.360	1.00	23.67	C
ATOM	499	CD2	TYR	G	217	19.496	-29.460	80.979	1.00	23.26	C
ATOM	500	CE1	TYR	G	217	17.638	-29.031	78.967	1.00	24.46	C
ATOM	501	CE2	TYR	G	217	19.179	-28.166	80.594	1.00	24.32	C
ATOM	502	CZ	TYR	G	217	18.247	-27.961	79.589	1.00	24.69	C
ATOM	503	OH	TYR	G	217	17.909	-26.690	79.227	1.00	24.29	O
ATOM	504	N	CYS	G	218	16.870	-34.575	80.641	1.00	24.27	N
ATOM	505	CA	CYS	G	218	16.695	-35.995	80.388	1.00	24.62	C
ATOM	506	C	CYS	G	218	17.113	-36.358	78.972	1.00	22.83	C
ATOM	507	O	CYS	G	218	17.567	-35.500	78.214	1.00	24.72	O
ATOM	508	CB	CYS	G	218	15.233	-36.354	80.639	1.00	26.38	C
ATOM	509	SG	CYS	G	218	14.704	-35.817	82.294	1.00	31.63	S
ATOM	510	N	ALA	G	219	16.974	-37.631	78.624	1.00	18.93	N
ATOM	511	CA	ALA	G	219	17.339	-38.109	77.294	1.00	16.07	C
ATOM	512	C	ALA	G	219	16.527	-37.448	76.171	1.00	13.63	C
ATOM	513	O	ALA	G	219	15.300	-37.319	76.257	1.00	13.39	O
ATOM	514	CB	ALA	G	219	17.195	-39.629	77.229	1.00	14.92	C
ATOM	515	N	PRO	G	220	17.219	-36.938	75.149	1.00	11.01	N
ATOM	516	CA	PRO	G	220	16.594	-36.283	74.001	1.00	11.11	C
ATOM	517	C	PRO	G	220	16.334	-37.262	72.860	1.00	13.18	C
ATOM	518	O	PRO	G	220	17.280	-37.698	72.182	1.00	13.29	O
ATOM	519	CB	PRO	G	220	17.643	-35.274	73.593	1.00	8.89	C
ATOM	520	CG	PRO	G	220	18.900	-36.045	73.827	1.00	7.54	C
ATOM	521	CD	PRO	G	220	18.667	-36.677	75.172	1.00	8.50	C
ATOM	522	N	ALA	G	221	15.061	-37.602	72.649	1.00	13.29	N
ATOM	523	CA	ALA	G	221	14.651	-38.512	71.579	1.00	12.43	C
ATOM	524	C	ALA	G	221	15.384	-39.856	71.586	1.00	13.18	C
ATOM	525	O	ALA	G	221	15.643	-40.442	72.651	1.00	14.79	O
ATOM	526	CB	ALA	G	221	14.820	-37.820	70.216	1.00	11.39	C
ATOM	527	N	GLY	G	222	15.702	-40.351	70.394	1.00	10.84	N
ATOM	528	CA	GLY	G	222	16.400	-41.612	70.290	1.00	11.36	C
ATOM	529	C	GLY	G	222	17.867	-41.511	70.656	1.00	9.70	C
ATOM	530	O	GLY	G	222	18.721	-41.916	69.861	1.00	10.63	O

FIG. 53-16

ATOM	532	CA	PHE	G	223	19.496	-40.809	72.373	1.00	8.42	C
ATOM	533	C	PHE	G	223	19.456	-41.268	73.828	1.00	9.49	C
ATOM	534	O	PHE	G	223	18.366	-41.488	74.378	1.00	10.19	O
ATOM	535	CB	PHE	G	223	19.896	-39.331	72.344	1.00	10.62	C
ATOM	536	CG	PHE	G	223	20.232	-38.807	70.979	1.00	10.55	C
ATOM	537	CD1	PHE	G	223	19.231	-38.447	70.084	1.00	11.49	C
ATOM	538	CD2	PHE	G	223	21.560	-38.694	70.579	1.00	12.49	C
ATOM	539	CE1	PHE	G	223	19.550	-37.980	68.805	1.00	12.26	C
ATOM	540	CE2	PHE	G	223	21.892	-38.228	69.305	1.00	12.26	C
ATOM	541	CZ	PHE	G	223	20.884	-37.872	68.416	1.00	11.74	C
ATOM	542	N	ALA	G	224	20.622	-41.402	74.459	1.00	9.64	N
ATOM	543	CA	ALA	G	224	20.696	-41.822	75.860	1.00	12.19	C
ATOM	544	C	ALA	G	224	21.767	-41.039	76.600	1.00	14.07	C
ATOM	545	O	ALA	G	224	22.819	-40.756	76.040	1.00	16.11	O
ATOM	546	CB	ALA	G	224	20.991	-43.300	75.959	1.00	13.88	C
ATOM	547	N	ILE	G	225	21.489	-40.660	77.843	1.00	15.13	N
ATOM	548	CA	ILE	G	225	22.460	-39.919	78.636	1.00	16.80	C
ATOM	549	C	ILE	G	225	23.354	-40.919	79.359	1.00	17.78	C
ATOM	550	O	ILE	G	225	22.861	-41.867	79.972	1.00	17.14	O
ATOM	551	CB	ILE	G	225	21.776	-38.988	79.680	1.00	16.89	C
ATOM	552	CG1	ILE	G	225	20.894	-37.961	78.974	1.00	17.32	C
ATOM	553	CG2	ILE	G	225	22.823	-38.241	80.499	1.00	15.61	C
ATOM	554	CD1	ILE	G	225	20.244	-36.988	79.911	1.00	18.48	C
ATOM	555	N	LEU	G	226	24.665	-40.714	79.265	1.00	19.57	N
ATOM	556	CA	LEU	G	226	25.647	-41.586	79.909	1.00	20.91	C
ATOM	557	C	LEU	G	226	26.440	-40.841	80.973	1.00	24.07	C
ATOM	558	O	LEU	G	226	27.391	-40.125	80.655	1.00	25.41	O
ATOM	559	CB	LEU	G	226	26.626	-42.145	78.877	1.00	18.80	C
ATOM	560	CG	LEU	G	226	26.421	-43.565	78.356	1.00	17.77	C
ATOM	561	CD1	LEU	G	226	25.136	-43.665	77.576	1.00	18.13	C
ATOM	562	CD2	LEU	G	226	27.594	-43.943	77.483	1.00	18.28	C
ATOM	563	N	LYS	G	227	26.073	-41.037	82.237	1.00	26.52	N
ATOM	564	CA	LYS	G	227	26.762	-40.383	83.342	1.00	27.94	C
ATOM	565	C	LYS	G	227	28.046	-41.125	83.675	1.00	29.17	C
ATOM	566	O	LYS	G	227	28.042	-42.351	83.782	1.00	28.73	O
ATOM	567	CB	LYS	G	227	25.871	-40.345	84.596	1.00	27.90	C
ATOM	568	CG	LYS	G	227	26.571	-39.821	85.871	1.00	29.64	C
ATOM	569	CD	LYS	G	227	25.679	-39.912	87.113	1.00	32.29	C
ATOM	570	CE	LYS	G	227	24.456	-39.001	86.999	1.00	34.48	C
ATOM	571	NZ	LYS	G	227	23.364	-39.285	87.981	1.00	34.38	N
ATOM	572	N	CYS	G	228	29.156	-40.402	83.769	1.00	30.76	N
ATOM	573	CA	CYS	G	228	30.406	-41.034	84.164	1.00	31.72	C
ATOM	574	C	CYS	G	228	30.354	-41.009	85.688	1.00	31.86	C
ATOM	575	O	CYS	G	228	30.128	-39.947	86.288	1.00	31.34	O
ATOM	576	CB	CYS	G	228	31.630	-40.254	83.684	1.00	32.88	C
ATOM	577	SG	CYS	G	228	33.191	-41.021	84.247	1.00	35.47	S
ATOM	578	N	ASN	G	229	30.543	-42.169	86.307	1.00	32.07	N
ATOM	579	CA	ASN	G	229	30.487	-42.279	87.761	1.00	32.72	C
ATOM	580	C	ASN	G	229	31.832	-42.135	88.457	1.00	34.60	C
ATOM	581	O	ASN	G	229	31.911	-42.205	89.686	1.00	35.58	O
ATOM	582	CB	ASN	G	229	29.826	-43.590	88.153	1.00	29.60	C
ATOM	583	CG	ASN	G	229	28.562	-43.849	87.372	1.00	27.66	C
ATOM	584	OD1	ASN	G	229	28.577	-44.573	86.383	1.00	29.57	O
ATOM	585	ND2	ASN	G	229	27.465	-43.236	87.788	1.00	25.67	N
ATOM	586	N	ASN	G	230	32.894	-41.963	87.676	1.00	36.32	N
ATOM	587	CA	ASN	G	230	34.235	-41.791	88.233	1.00	38.29	C
ATOM	588	C	ASN	G	230	34.178	-40.551	89.128	1.00	39.43	C
ATOM	589	O	ASN	G	230	34.082	-39.421	88.631	1.00	40.23	O
ATOM	590	CB	ASN	G	230	35.249	-41.587	87.101	1.00	39.40	C
ATOM	591	CG	ASN	G	230	36.676	-41.423	87.602	1.00	41.01	C
ATOM	592	OD1	ASN	G	230	36.909	-41.063	88.758	1.00	42.26	O
ATOM	593	ND2	ASN	G	230	37.641	-41.688	86.730	1.00	41.03	N
ATOM	594	N	LYS	G	231	34.212	-40.776	90.442	1.00	39.89	N
ATOM	595	CA	LYS	G	231	34.130	-39.706	91.447	1.00	39.44	C
ATOM	596	C	LYS	G	231	34.979	-38.480	91.139	1.00	38.08	C
ATOM	597	O	LYS	G	231	34.615	-37.360	91.500	1.00	36.75	O
ATOM	598	CB	LYS	G	231	34.504	-40.238	92.835	1.00	41.08	C
ATOM	599	CG	LYS	G	231	35.963	-40.671	92.968	1.00	44.34	C
ATOM	600	CD	LYS	G	231	36.306	-41.090	94.396	1.00	45.89	C
ATOM	601	CE	LYS	G	231	37.782	-41.470	94.521	1.00	47.71	C

FIG. 53-17

ATOM	603	N	THR	G	232	36.099	-38.700	90.460	1.00	37.10	N
ATOM	604	CA	THR	G	232	37.012	-37.625	90.110	1.00	36.36	C
ATOM	605	C	THR	G	232	37.277	-37.596	88.605	1.00	36.66	C
ATOM	606	O	THR	G	232	38.435	-37.552	88.169	1.00	37.42	O
ATOM	607	CB	THR	G	232	38.345	-37.802	90.840	1.00	35.93	C
ATOM	608	OG1	THR	G	232	38.102	-38.234	92.189	1.00	35.22	O
ATOM	609	CG2	THR	G	232	39.117	-36.492	90.861	1.00	37.20	C
ATOM	610	N	PHE	G	233	36.217	-37.654	87.802	1.00	35.64	N
ATOM	611	CA	PHE	G	233	36.398	-37.616	86.357	1.00	34.71	C
ATOM	612	C	PHE	G	233	36.969	-36.249	86.011	1.00	34.94	C
ATOM	613	O	PHE	G	233	36.451	-35.214	86.442	1.00	35.73	O
ATOM	614	CB	PHE	G	233	35.078	-37.847	85.622	1.00	33.02	C
ATOM	615	CG	PHE	G	233	35.241	-38.061	84.142	1.00	29.97	C
ATOM	616	CD1	PHE	G	233	36.468	-38.461	83.612	1.00	28.03	C
ATOM	617	CD2	PHE	G	233	34.174	-37.856	83.279	1.00	27.59	C
ATOM	618	CE1	PHE	G	233	36.625	-38.650	82.250	1.00	27.32	C
ATOM	619	CE2	PHE	G	233	34.322	-38.043	81.919	1.00	26.38	C
ATOM	620	CZ	PHE	G	233	35.547	-38.440	81.400	1.00	26.71	C
ATOM	621	N	ASN	G	234	38.033	-36.247	85.225	1.00	34.87	N
ATOM	622	CA	ASN	G	234	38.697	-35.012	84.873	1.00	35.27	C
ATOM	623	C	ASN	G	234	38.655	-34.658	83.394	1.00	35.04	C
ATOM	624	O	ASN	G	234	39.563	-34.971	82.630	1.00	33.89	O
ATOM	625	CB	ASN	G	234	40.123	-35.058	85.422	1.00	38.76	C
ATOM	626	CG	ASN	G	234	40.998	-33.931	84.914	1.00	42.99	C
ATOM	627	OD1	ASN	G	234	40.748	-32.752	85.180	1.00	42.47	O
ATOM	628	ND2	ASN	G	234	42.059	-34.309	84.204	1.00	47.05	N
ATOM	629	N	GLY	G	235	37.541	-34.047	83.007	1.00	36.12	N
ATOM	630	CA	GLY	G	235	37.333	-33.596	81.643	1.00	36.47	C
ATOM	631	C	GLY	G	235	37.286	-34.625	80.532	1.00	37.20	C
ATOM	632	O	GLY	G	235	36.373	-35.448	80.450	1.00	36.74	O
ATOM	633	N	THR	G	236	38.265	-34.517	79.643	1.00	38.34	N
ATOM	634	CA	THR	G	236	38.400	-35.386	78.484	1.00	38.15	C
ATOM	635	C	THR	G	236	39.055	-36.704	78.885	1.00	37.90	C
ATOM	636	O	THR	G	236	39.874	-36.744	79.805	1.00	37.08	O
ATOM	637	CB	THR	G	236	39.275	-34.700	77.416	1.00	37.38	C
ATOM	638	OG1	THR	G	236	38.882	-33.327	77.293	1.00	38.47	O
ATOM	639	CG2	THR	G	236	39.130	-35.379	76.069	1.00	36.15	C
ATOM	640	N	GLY	G	237	38.685	-37.781	78.201	1.00	38.40	N
ATOM	641	CA	GLY	G	237	39.278	-39.068	78.504	1.00	38.38	C
ATOM	642	C	GLY	G	237	38.295	-40.218	78.510	1.00	39.07	C
ATOM	643	O	GLY	G	237	37.075	-40.016	78.501	1.00	38.90	O
ATOM	644	N	PRO	G	238	38.809	-41.456	78.508	1.00	39.11	N
ATOM	645	CA	PRO	G	238	37.973	-42.653	78.513	1.00	39.26	C
ATOM	646	C	PRO	G	238	37.466	-42.981	79.913	1.00	39.29	C
ATOM	647	O	PRO	G	238	38.191	-43.555	80.733	1.00	39.99	O
ATOM	648	CB	PRO	G	238	38.924	-43.722	77.981	1.00	39.01	C
ATOM	649	CG	PRO	G	238	40.222	-43.310	78.557	1.00	38.17	C
ATOM	650	CD	PRO	G	238	40.231	-41.811	78.355	1.00	38.34	C
ATOM	651	N	CYS	G	239	36.240	-42.559	80.205	1.00	38.74	N
ATOM	652	CA	CYS	G	239	35.639	-42.827	81.502	1.00	37.11	C
ATOM	653	C	CYS	G	239	35.481	-44.330	81.670	1.00	36.78	C
ATOM	654	O	CYS	G	239	34.889	-45.002	80.824	1.00	36.13	O
ATOM	655	CB	CYS	G	239	34.269	-42.156	81.622	1.00	36.43	C
ATOM	656	SG	CYS	G	239	33.333	-42.688	83.095	1.00	34.24	S
ATOM	657	N	THR	G	240	36.023	-44.853	82.761	1.00	37.49	N
ATOM	658	CA	THR	G	240	35.931	-46.274	83.050	1.00	37.98	C
ATOM	659	C	THR	G	240	34.533	-46.598	83.586	1.00	37.13	C
ATOM	660	O	THR	G	240	33.684	-47.130	82.868	1.00	37.18	O
ATOM	661	CB	THR	G	240	37.003	-46.699	84.081	1.00	39.11	C
ATOM	662	OG1	THR	G	240	37.034	-45.752	85.157	1.00	39.76	O
ATOM	663	CG2	THR	G	240	38.379	-46.767	83.430	1.00	39.56	C
ATOM	664	N	ASN	G	241	34.291	-46.228	84.839	1.00	36.08	N
ATOM	665	CA	ASN	G	241	33.013	-46.457	85.494	1.00	35.12	C
ATOM	666	C	ASN	G	241	31.985	-45.476	84.924	1.00	34.97	C
ATOM	667	O	ASN	G	241	32.108	-44.266	85.120	1.00	35.71	O
ATOM	668	CB	ASN	G	241	33.185	-46.253	87.001	1.00	34.78	C
ATOM	669	CG	ASN	G	241	31.956	-46.648	87.795	1.00	35.17	C
ATOM	670	OD1	ASN	G	241	30.847	-46.703	87.262	1.00	35.56	O
ATOM	671	ND2	ASN	G	241	32.149	-46.926	89.081	1.00	33.79	N
ATOM	672	N	VAL	G	242	30.983	-45.997	84.221	1.00	34.43	N

FIG. 53-18

ATOM	674	C	VAL	G	242	28.633	-45.926	83.469	1.00	34.85	C
ATOM	675	O	VAL	G	242	28.630	-47.158	83.403	1.00	35.99	O
ATOM	676	CB	VAL	G	242	30.401	-44.674	82.193	1.00	34.41	C
ATOM	677	CG1	VAL	G	242	30.835	-45.841	81.336	1.00	34.06	C
ATOM	678	CG2	VAL	G	242	29.284	-43.929	81.506	1.00	35.80	C
ATOM	679	N	SER	G	243	27.520	-45.197	83.422	1.00	34.24	N
ATOM	680	CA	SER	G	243	26.202	-45.814	83.306	1.00	33.06	C
ATOM	681	C	SER	G	243	25.149	-44.908	82.678	1.00	31.78	C
ATOM	682	O	SER	G	243	25.223	-43.680	82.779	1.00	32.45	O
ATOM	683	CB	SER	G	243	25.730	-46.294	84.682	1.00	34.26	C
ATOM	684	OG	SER	G	243	25.920	-45.301	85.680	1.00	34.99	O
ATOM	685	N	THR	G	244	24.178	-45.523	82.013	1.00	29.73	N
ATOM	686	CA	THR	G	244	23.100	-44.794	81.366	1.00	29.06	C
ATOM	687	C	THR	G	244	22.137	-44.262	82.415	1.00	29.76	C
ATOM	688	O	THR	G	244	21.936	-44.894	83.446	1.00	29.94	O
ATOM	689	CB	THR	G	244	22.337	-45.694	80.375	1.00	28.55	C
ATOM	690	OG1	THR	G	244	23.162	-45.975	79.238	1.00	27.22	O
ATOM	691	CG2	THR	G	244	21.073	-45.021	79.906	1.00	30.50	C
ATOM	692	N	VAL	G	245	21.581	-43.079	82.162	1.00	30.22	N
ATOM	693	CA	VAL	G	245	20.629	-42.439	83.068	1.00	28.10	C
ATOM	694	C	VAL	G	245	19.507	-41.832	82.244	1.00	27.35	C
ATOM	695	O	VAL	G	245	19.677	-41.544	81.056	1.00	26.22	O
ATOM	696	CB	VAL	G	245	21.281	-41.312	83.919	1.00	26.91	C
ATOM	697	CG1	VAL	G	245	22.250	-41.890	84.926	1.00	28.47	C
ATOM	698	CG2	VAL	G	245	22.000	-40.321	83.036	1.00	26.25	C
ATOM	699	N	GLN	G	246	18.352	-41.661	82.874	1.00	27.28	N
ATOM	700	CA	GLN	G	246	17.197	-41.086	82.202	1.00	28.75	C
ATOM	701	C	GLN	G	246	17.335	-39.566	82.151	1.00	29.05	C
ATOM	702	O	GLN	G	246	16.933	-38.930	81.174	1.00	28.66	O
ATOM	703	CB	GLN	G	246	15.913	-41.469	82:934	1.00	30.26	C
ATOM	704	CG	GLN	G	246	14.656	-41.135	82.163	1.00	33.92	C
ATOM	705	CD	GLN	G	246	14.473	-42.015	80.944	1.00	35.79	C
ATOM	706	OE1	GLN	G	246	14.017	-43.155	81.053	1.00	37.71	O
ATOM	707	NE2	GLN	G	246	14.820	-41.489	79.772	1.00	35.44	N
ATOM	708	N	CYS	G	247	17.900	-38.997	83.215	1.00	29.31	N
ATOM	709	CA	CYS	G	247	18.125	-37.556	83.317	1.00	29.67	C
ATOM	710	C	CYS	G	247	19.424	-37.342	84.095	1.00	28.79	C
ATOM	711	O	CYS	G	247	19.809	-38.184	84.910	1.00	29.02	O
ATOM	712	CB	CYS	G	247	16.966	-36.870	84.053	1.00	30.99	C
ATOM	713	SG	CYS	G	247	15.297	-37.346	83.488	1.00	32.88	S
ATOM	714	N	THR	G	248	20.087	-36.215	83.840	1.00	27.61	N
ATOM	715	CA	THR	G	248	21.350	-35.860	84.490	1.00	25.20	C
ATOM	716	C	THR	G	248	21.286	-35.759	86.025	1.00	23.90	C
ATOM	717	O	THR	G	248	21.641	-36.718	86.732	1.00	25.55	O
ATOM	718	CB	THR	G	248	21.897	-34.551	83.898	1.00	24.29	C
ATOM	719	OG1	THR	G	248	20.890	-33.533	83.968	1.00	24.48	O
ATOM	720	CG2	THR	G	248	22.282	-34.758	82.444	1.00	23.90	C
ATOM	721	N	HIS	G	249	20.923	-34.581	86.526	1.00	21.13	N
ATOM	722	CA	HIS	G	249	20.779	-34.311	87.960	1.00	19.07	C
ATOM	723	C	HIS	G	249	20.168	-32.918	88.142	1.00	16.85	C
ATOM	724	O	HIS	G	249	19.735	-32.307	87.161	1.00	15.06	O
ATOM	725	CB	HIS	G	249	22.104	-34.470	88.738	1.00	21.24	C
ATOM	726	CG	HIS	G	249	23.159	-33.461	88.399	1.00	21.64	C
ATOM	727	ND1	HIS	G	249	23.445	-33.112	87.106	1.00	23.08	N
ATOM	728	CD2	HIS	G	249	24.025	-32.825	89.232	1.00	21.09	C
ATOM	729	CE1	HIS	G	249	24.467	-32.282	87.173	1.00	23.31	C
ATOM	730	NE2	HIS	G	249	24.853	-32.079	88.439	1.00	20.74	N
ATOM	731	N	GLY	G	250	20.029	-32.462	89.386	1.00	13.85	N
ATOM	732	CA	GLY	G	250	19.436	-31.154	89.630	1.00	11.77	C
ATOM	733	C	GLY	G	250	20.382	-30.011	89.355	1.00	9.55	C
ATOM	734	O	GLY	G	250	21.061	-29.553	90.265	1.00	7.84	O
ATOM	735	N	ILE	G	251	20.371	-29.512	88.122	1.00	8.82	N
ATOM	736	CA	ILE	G	251	21.274	-28.447	87.718	1.00	10.81	C
ATOM	737	C	ILE	G	251	20.680	-27.060	87.930	1.00	13.34	C
ATOM	738	O	ILE	G	251	19.649	-26.739	87.351	1.00	14.54	O
ATOM	739	CB	ILE	G	251	21.630	-28.564	86.220	1.00	9.66	C
ATOM	740	CG1	ILE	G	251	21.804	-30.025	85.810	1.00	10.10	C
ATOM	741	CG2	ILE	G	251	22.922	-27.827	85.932	1.00	11.25	C
ATOM	742	CD1	ILE	G	251	21.969	-30.217	84.306	1.00	10.97	C
ATOM	743	N	ARG	G	252	21.310	-26.242	88.762	1.00	14.65	N

FIG. 53-19

ATOM	745	C	ARG	G	252	21.536	-23.902	88.040	1.00	15.18	C
ATOM	746	O	ARG	G	252	22.729	-23.612	88.184	1.00	14.72	O
ATOM	747	CB	ARG	G	252	21.089	-24.447	90.437	1.00	16.34	C
ATOM	748	CG	ARG	G	252	19.816	-24.400	91.267	1.00	18.59	C
ATOM	749	CD	ARG	G	252	20.048	-23.675	92.571	1.00	20.27	C
ATOM	750	NE	ARG	G	252	21.125	-24.274	93.352	1.00	21.75	N
ATOM	751	CZ	ARG	G	252	21.095	-24.399	94.671	1.00	22.91	C
ATOM	752	NH1	ARG	G	252	20.035	-23.967	95.347	1.00	23.31	N
ATOM	753	NH2	ARG	G	252	22.125	-24.947	95.307	1.00	23.29	N
ATOM	754	N	PRO	G	253	20.794	-23.380	87.050	1.00	14.19	N
ATOM	755	CA	PRO	G	253	21.369	-22.446	86.082	1.00	15.88	C
ATOM	756	C	PRO	G	253	21.631	-21.059	86.659	1.00	17.45	C
ATOM	757	O	PRO	G	253	20.769	-20.184	86.640	1.00	18.70	O
ATOM	758	CB	PRO	G	253	20.320	-22.430	84.978	1.00	15.49	C
ATOM	759	CG	PRO	G	253	19.040	-22.604	85.746	1.00	14.37	C
ATOM	760	CD	PRO	G	253	19.391	-23.683	86.722	1.00	13.38	C
ATOM	761	N	VAL	G	254	22.821	-20.868	87.205	1.00	17.92	N
ATOM	762	CA	VAL	G	254	23.166	-19.583	87.786	1.00	17.08	C
ATOM	763	C	VAL	G	254	24.073	-18.852	86.828	1.00	16.36	C
ATOM	764	O	VAL	G	254	25.088	-19.396	86.392	1.00	18.64	O
ATOM	765	CB	VAL	G	254	23.897	-19.744	89.135	1.00	18.77	C
ATOM	766	CG1	VAL	G	254	24.303	-18.376	89.680	1.00	20.07	C
ATOM	767	CG2	VAL	G	254	23.013	-20.485	90.136	1.00	15.73	C
ATOM	768	N	VAL	G	255	23.654	-17.660	86.423	1.00	13.80	N
ATOM	769	CA	VAL	G	255	24.459	-16.842	85.528	1.00	11.88	C
ATOM	770	C	VAL	G	255	25.293	-15.902	86.398	1.00	11.33	C
ATOM	771	O	VAL	G	255	24.753	-15.203	87.265	1.00	11.59	O
ATOM	772	CB	VAL	G	255	23.582	-16.030	84.582	1.00	11.26	C
ATOM	773	CG1	VAL	G	255	24.422	-14.993	83.857	1.00	12.22	C
ATOM	774	CG2	VAL	G	255	22.905	-16.957	83.591	1.00	8.16	C
ATOM	775	N	SER	G	256	26.602	-15.900	86.184	1.00	9.34	N
ATOM	776	CA	SER	G	256	27.488	-15.065	86.974	1.00	9.65	C
ATOM	777	C	SER	G	256	28.901	-15.234	86.447	1.00	8.51	C
ATOM	778	O	SER	G	256	29.167	-16.172	85.692	1.00	7.45	O
ATOM	779	CB	SER	G	256	27.416	-15.499	88.440	1.00	11.83	C
ATOM	780	OG	SER	G	256	27.666	-16.894	88.563	1.00	16.05	O
ATOM	781	N	THR	G	257	29.806	-14.344	86.849	1.00	6.62	N
ATOM	782	CA	THR	G	257	31.186	-14.409	86.388	1.00	7.04	C
ATOM	783	C	THR	G	257	32.209	-14.728	87.463	1.00	8.38	C
ATOM	784	O	THR	G	257	31.963	-14.529	88.654	1.00	6.92	O
ATOM	785	CB	THR	G	257	31.596	-13.104	85.702	1.00	6.93	C
ATOM	786	OG1	THR	G	257	31.300	-11.999	86.574	1.00	6.69	O
ATOM	787	CG2	THR	G	257	30.855	-12.950	84.386	1.00	4.16	C
ATOM	788	N	GLN	G	258	33.377	-15.190	87.010	1.00	10.72	N
ATOM	789	CA	GLN	G	258	34.517	-15.569	87.852	1.00	13.00	C
ATOM	790	C	GLN	G	258	34.282	-16.449	89.076	1.00	13.60	C
ATOM	791	O	GLN	G	258	35.225	-17.050	89.590	1.00	12.26	O
ATOM	792	CB	GLN	G	258	35.425	-14.360	88.187	1.00	16.33	C
ATOM	793	CG	GLN	G	258	34.769	-13.073	88.686	1.00	18.73	C
ATOM	794	CD	GLN	G	258	35.736	-11.885	88.689	1.00	22.36	C
ATOM	795	OE1	GLN	G	258	36.009	-11.297	89.730	1.00	26.27	O
ATOM	796	NE2	GLN	G	258	36.249	-11.530	87.522	1.00	22.75	N
ATOM	797	N	LEU	G	259	33.025	-16.608	89.482	1.00	14.36	N
ATOM	798	CA	LEU	G	259	32.687	-17.423	90.637	1.00	14.56	C
ATOM	799	C	LEU	G	259	31.411	-18.193	90.312	1.00	15.43	C
ATOM	800	O	LEU	G	259	30.372	-17.603	90.038	1.00	14.37	O
ATOM	801	CB	LEU	G	259	32.468	-16.553	91.885	1.00	13.53	C
ATOM	802	CG	LEU	G	259	33.520	-15.542	92.381	1.00	14.36	C
ATOM	803	CD1	LEU	G	259	32.979	-14.812	93.598	1.00	13.95	C
ATOM	804	CD2	LEU	G	259	34.834	-16.214	92.727	1.00	12.89	C
ATOM	805	N	LEU	G	260	31.544	-19.514	90.233	1.00	17.80	N
ATOM	806	CA	LEU	G	260	30.426	-20.411	89.967	1.00	16.61	C
ATOM	807	C	LEU	G	260	29.751	-20.526	91.328	1.00	16.85	C
ATOM	808	O	LEU	G	260	30.418	-20.767	92.343	1.00	16.91	O
ATOM	809	CB	LEU	G	260	30.944	-21.777	89.505	1.00	15.05	C
ATOM	810	CG	LEU	G	260	31.548	-21.902	88.103	1.00	12.93	C
ATOM	811	CD1	LEU	G	260	32.443	-23.115	88.006	1.00	9.99	C
ATOM	812	CD2	LEU	G	260	30.436	-21.995	87.083	1.00	14.84	C
ATOM	813	N	LEU	G	261	28.438	-20.355	91.357	1.00	16.28	N
ATOM	814	CA	LEU	G	261	27.714	-20.387	92.619	1.00	15.45	C

FIG. 53-20

ATOM	816	O	LEU	G	261	26.055	-21.719	91.530	1.00	15.07	O
ATOM	817	CB	LEU	G	261	27.155	-18.994	92.941	1.00	15.44	C
ATOM	818	CG	LEU	G	261	27.903	-17.709	92.562	1.00	14.64	C
ATOM	819	CD1	LEU	G	261	26.995	-16.531	92.836	1.00	15.56	C
ATOM	820	CD2	LEU	G	261	29.208	-17.580	93.328	1.00	14.51	C
ATOM	821	N	ASN	G	262	26.091	-21.722	93.795	1.00	14.73	N
ATOM	822	CA	ASN	G	262	24.955	-22.617	93.986	1.00	15.35	C
ATOM	823	C	ASN	G	262	24.966	-23.881	93.128	1.00	16.77	C
ATOM	824	O	ASN	G	262	23.895	-24.406	92.778	1.00	14.61	O
ATOM	825	CB	ASN	G	262	23.655	-21.840	93.763	1.00	13.25	C
ATOM	826	CG	ASN	G	262	23.276	-21.004	94.953	1.00	14.34	C
ATOM	827	OD1	ASN	G	262	24.149	-20.476	95.649	1.00	13.74	O
ATOM	828	ND2	ASN	G	262	21.974	-20.958	95.249	1.00	19.13	N
ATOM	829	N	GLY	G	263	26.162	-24.430	92.910	1.00	18.74	N
ATOM	830	CA	GLY	G	263	26.297	-25.613	92.070	1.00	20.11	C
ATOM	831	C	GLY	G	263	26.893	-26.866	92.695	1.00	20.38	C
ATOM	832	O	GLY	G	263	26.976	-26.990	93.918	1.00	18.64	O
ATOM	833	N	SER	G	264	27.340	-27.783	91.839	1.00	22.57	N
ATOM	834	CA	SER	G	264	27.920	-29.055	92.272	1.00	24.43	C
ATOM	835	C	SER	G	264	29.383	-28.986	92.685	1.00	24.80	C
ATOM	836	O	SER	G	264	30.222	-28.469	91.947	1.00	26.75	O
ATOM	837	CB	SER	G	264	27.731	-30.114	91.181	1.00	24.18	C
ATOM	838	OG	SER	G	264	28.390	-31.332	91.492	1.00	25.32	O
ATOM	839	N	LEU	G	265	29.679	-29.569	93.842	1.00	24.24	N
ATOM	840	CA	LEU	G	265	31.026	-29.599	94.405	1.00	24.88	C
ATOM	841	C	LEU	G	265	31.707	-30.915	94.056	1.00	26.63	C
ATOM	842	O	LEU	G	265	31.068	-31.863	93.581	1.00	28.11	O
ATOM	843	CB	LEU	G	265	30.971	-29.520	95.936	1.00	23.01	C
ATOM	844	CG	LEU	G	265	30.425	-28.329	96.727	1.00	21.06	C
ATOM	845	CD1	LEU	G	265	30.318	-28.728	98.173	1.00	19.70	C
ATOM	846	CD2	LEU	G	265	31.333	-27.131	96.597	1.00	19.59	C
ATOM	847	N	ALA	G	266	33.006	-30.980	94.321	1.00	26.39	N
ATOM	848	CA	ALA	G	266	33.755	-32.200	94.089	1.00	27.04	C
ATOM	849	C	ALA	G	266	33.572	-33.011	95.364	1.00	28.11	C
ATOM	850	O	ALA	G	266	33.583	-32.463	96.472	1.00	26.76	O
ATOM	851	CB	ALA	G	266	35.224	-31.898	93.860	1.00	26.32	C
ATOM	852	N	GLU	G	267	33.364	-34.313	95.216	1.00	30.45	N
ATOM	853	CA	GLU	G	267	33.183	-35.150	96.390	1.00	31.74	C
ATOM	854	C	GLU	G	267	34.493	-35.663	96.959	1.00	31.08	C
ATOM	855	O	GLU	G	267	34.528	-36.149	98.087	1.00	31.50	O
ATOM	856	CB	GLU	G	267	32.215	-36.296	96.108	1.00	33.74	C
ATOM	857	CG	GLU	G	267	32.572	-37.169	94.930	1.00	36.70	C
ATOM	858	CD	GLU	G	267	31.470	-38.154	94.615	1.00	38.49	C
ATOM	859	OE1	GLU	G	267	30.287	-37.741	94.642	1.00	38.38	O
ATOM	860	OE2	GLU	G	267	31.781	-39.336	94.346	1.00	40.34	O
ATOM	861	N	GLU	G	268	35.569	-35.537	96.193	1.00	30.63	N
ATOM	862	CA	GLU	G	268	36.871	-35.993	96.661	1.00	31.06	C
ATOM	863	C	GLU	G	268	37.859	-34.887	96.982	1.00	30.70	C
ATOM	864	O	GLU	G	268	38.087	-34.567	98.149	1.00	31.59	O
ATOM	865	CB	GLU	G	268	37.475	-36.972	95.666	1.00	30.64	C
ATOM	866	CG	GLU	G	268	37.182	-38.400	96.033	1.00	32.42	C
ATOM	867	CD	GLU	G	268	37.983	-38.864	97.234	1.00	34.32	C
ATOM	868	OE1	GLU	G	268	39.142	-39.287	97.039	1.00	33.80	O
ATOM	869	OE2	GLU	G	268	37.446	-38.823	98.359	1.00	36.47	O
ATOM	870	N	GLU	G	269	38.475	-34.330	95.947	1.00	29.74	N
ATOM	871	CA	GLU	G	269	39.443	-33.259	96.116	1.00	28.78	C
ATOM	872	C	GLU	G	269	39.107	-32.188	95.099	1.00	27.43	C
ATOM	873	O	GLU	G	269	38.184	-32.356	94.296	1.00	26.47	O
ATOM	874	CB	GLU	G	269	40.858	-33.767	95.847	1.00	30.51	C
ATOM	875	CG	GLU	G	269	41.339	-34.857	96.781	1.00	34.12	C
ATOM	876	CD	GLU	G	269	42.556	-35.568	96.235	1.00	37.29	C
ATOM	877	OE1	GLU	G	269	42.376	-36.543	95.470	1.00	38.77	O
ATOM	878	OE2	GLU	G	269	43.688	-35.132	96.539	1.00	38.33	O
ATOM	879	N	VAL	G	270	39.863	-31.093	95.133	1.00	25.65	N
ATOM	880	CA	VAL	G	270	39.665	-29.995	94.199	1.00	22.37	C
ATOM	881	C	VAL	G	270	40.100	-30.507	92.830	1.00	20.77	C
ATOM	882	O	VAL	G	270	41.216	-31.019	92.677	1.00	21.12	O
ATOM	883	CB	VAL	G	270	40.524	-28.759	94.579	1.00	21.80	C
ATOM	884	CG1	VAL	G	270	40.193	-27.581	93.666	1.00	19.80	C
ATOM	885	CG2	VAL	G	270	40.299	-28.378	96.035	1.00	21.76	C

FIG. 53-21

ATOM	887	CA	VAL	G	271	39.487	-30.856	90.500	1.00	15.81	C
ATOM	888	C	VAL	G	271	39.389	-29.664	89.562	1.00	15.48	C
ATOM	889	O	VAL	G	271	38.424	-28.910	89.618	1.00	15.34	O
ATOM	890	CB	VAL	G	271	38.475	-31.916	90.036	1.00	14.93	C
ATOM	891	CG1	VAL	G	271	38.854	-32.436	88.652	1.00	16.36	C
ATOM	892	CG2	VAL	G	271	38.413	-33.050	91.031	1.00	12.91	C
ATOM	893	N	ILE	G	272	40.387	-29.500	88.703	1.00	14.98	N
ATOM	894	CA	ILE	G	272	40.418	-28.402	87.744	1.00	15.27	C
ATOM	895	C	ILE	G	272	40.249	-29.029	86.367	1.00	14.98	C
ATOM	896	O	ILE	G	272	40.471	-30.223	86.202	1.00	17.63	O
ATOM	897	CB	ILE	G	272	41.765	-27.619	87.822	1.00	15.43	C
ATOM	898	CG1	ILE	G	272	42.943	-28.550	87.501	1.00	15.65	C
ATOM	899	CG2	ILE	G	272	41.930	-26.992	89.211	1.00	14.26	C
ATOM	900	CD1	ILE	G	272	44.307	-27.944	87.724	1.00	13.52	C
ATOM	901	N	ARG	G	273	39.839	-28.240	85.386	1.00	13.53	N
ATOM	902	CA	ARG	G	273	39.633	-28.743	84.039	1.00	12.31	C
ATOM	903	C	ARG	G	273	39.828	-27.640	83.000	1.00	13.14	C
ATOM	904	O	ARG	G	273	39.500	-26.476	83.241	1.00	12.25	O
ATOM	905	CB	ARG	G	273	38.244	-29.381	83.925	1.00	11.20	C
ATOM	906	CG	ARG	G	273	38.204	-30.836	84.392	1.00	12.42	C
ATOM	907	CD	ARG	G	273	36.795	-31.387	84.533	1.00	7.85	C
ATOM	908	NE	ARG	G	273	36.151	-30.834	85.711	1.00	8.24	N
ATOM	909	CZ	ARG	G	273	35.797	-31.538	86.786	1.00	6.73	C
ATOM	910	NH1	ARG	G	273	36.011	-32.851	86.846	1.00	2.00	N
ATOM	911	NH2	ARG	G	273	35.297	-30.898	87.839	1.00	6.75	N
ATOM	912	N	SER	G	274	40.421	-28.008	81.866	1.00	14.05	N
ATOM	913	CA	SER	G	274	40.685	-27.083	80.771	1.00	14.41	C
ATOM	914	C	SER	G	274	40.862	-27.881	79.498	1.00	16.49	C
ATOM	915	O	SER	G	274	41.250	-29.051	79.541	1.00	16.60	O
ATOM	916	CB	SER	G	274	41.959	-26.295	81.019	1.00	13.52	C
ATOM	917	OG	SER	G	274	42.300	-25.536	79.866	1.00	14.72	O
ATOM	918	N	VAL	G	275	40.588	-27.239	78.365	1.00	18.87	N
ATOM	919	CA	VAL	G	275	40.713	-27.881	77.061	1.00	20.86	C
ATOM	920	C	VAL	G	275	42.171	-28.111	76.797	1.00	21.77	C
ATOM	921	O	VAL	G	275	42.571	-29.156	76.288	1.00	22.15	O
ATOM	922	CB	VAL	G	275	40.208	-26.977	75.912	1.00	22.43	C
ATOM	923	CG1	VAL	G	275	40.314	-27.704	74.579	1.00	21.35	C
ATOM	924	CG2	VAL	G	275	38.784	-26.540	76.158	1.00	23.72	C
ATOM	925	N	ASN	G	276	42.968	-27.115	77.163	1.00	23.25	N
ATOM	926	CA	ASN	G	276	44.404	-27.151	76.937	1.00	23.21	C
ATOM	927	C	ASN	G	276	45.032	-26.306	78.024	1.00	22.58	C
ATOM	928	O	ASN	G	276	44.917	-25.081	77.997	1.00	23.34	O
ATOM	929	CB	ASN	G	276	44.690	-26.511	75.582	1.00	24.97	C
ATOM	930	CG	ASN	G	276	46.021	-26.925	74.999	1.00	26.93	C
ATOM	931	OD1	ASN	G	276	47.022	-27.103	75.710	1.00	26.46	O
ATOM	932	ND2	ASN	G	276	46.025	-27.059	73.678	1.00	27.04	N
ATOM	933	N	PHE	G	277	45.652	-26.961	78.999	1.00	21.99	N
ATOM	934	CA	PHE	G	277	46.296	-26.265	80.110	1.00	21.09	C
ATOM	935	C	PHE	G	277	47.529	-25.503	79.640	1.00	21.98	C
ATOM	936	O	PHE	G	277	48.088	-24.707	80.395	1.00	21.74	O
ATOM	937	CB	PHE	G	277	46.714	-27.258	81.202	1.00	20.81	C
ATOM	938	CG	PHE	G	277	45.567	-27.891	81.933	1.00	19.89	C
ATOM	939	CD1	PHE	G	277	45.015	-29.081	81.490	1.00	19.94	C
ATOM	940	CD2	PHE	G	277	45.059	-27.312	83.092	1.00	21.02	C
ATOM	941	CE1	PHE	G	277	43.974	-29.697	82.190	1.00	20.42	C
ATOM	942	CE2	PHE	G	277	44.013	-27.921	83.800	1.00	21.46	C
ATOM	943	CZ	PHE	G	277	43.474	-29.118	83.347	1.00	20.53	C
ATOM	944	N	THR	G	278	47.962	-25.760	78.404	1.00	22.61	N
ATOM	945	CA	THR	G	278	49.139	-25.110	77.829	1.00	23.71	C
ATOM	946	C	THR	G	278	48.835	-23.739	77.203	1.00	23.69	C
ATOM	947	O	THR	G	278	49.607	-22.787	77.355	1.00	22.77	O
ATOM	948	CB	THR	G	278	49.787	-26.001	76.748	1.00	26.18	C
ATOM	949	OG1	THR	G	278	49.862	-27.355	77.218	1.00	29.00	O
ATOM	950	CG2	THR	G	278	51.200	-25.505	76.428	1.00	28.03	C
ATOM	951	N	ASP	G	279	47.743	-23.665	76.449	1.00	23.78	N
ATOM	952	CA	ASP	G	279	47.338	-22.426	75.802	1.00	22.85	C
ATOM	953	C	ASP	G	279	46.767	-21.521	76.875	1.00	21.97	C
ATOM	954	O	ASP	G	279	45.656	-21.741	77.354	1.00	21.82	O
ATOM	955	CB	ASP	G	279	46.272	-22.710	74.736	1.00	25.27	C
ATOM	956	CG	ASP	G	279	45.708	-21.439	74.098	1.00	26.33	C

FIG. 53-22

ATOM	958	OD2	ASP	G	279	44.644	-21.532	73.433	1.00	24.54	O
ATOM	959	N	ASN	G	280	47.531	-20.503	77.248	1.00	20.54	N
ATOM	960	CA	ASN	G	280	47.116	-19.549	78.275	1.00	19.55	C
ATOM	961	C	ASN	G	280	45.782	-18.855	77.989	1.00	19.43	C
ATOM	962	O	ASN	G	280	45.151	-18.317	78.893	1.00	20.85	O
ATOM	963	CB	ASN	G	280	48.206	-18.493	78.499	1.00	17.41	C
ATOM	964	CG	ASN	G	280	48.596	-17.764	77.220	1.00	15.05	C
ATOM	965	OD1	ASN	G	280	47.840	-17.716	76.241	1.00	13.88	O
ATOM	966	ND2	ASN	G	280	49.792	-17.201	77.220	1.00	12.65	N
ATOM	967	N	ALA	G	281	45.355	-18.864	76.734	1.00	18.58	N
ATOM	968	CA	ALA	G	281	44.107	-18.223	76.349	1.00	16.85	C
ATOM	969	C	ALA	G	281	42.863	-18.972	76.786	1.00	16.69	C
ATOM	970	O	ALA	G	281	41.784	-18.389	76.828	1.00	17.95	O
ATOM	971	CB	ALA	G	281	44.072	-18.023	74.853	1.00	15.93	C
ATOM	972	N	LYS	G	282	43.012	-20.248	77.135	1.00	16.80	N
ATOM	973	CA	LYS	G	282	41.873	-21.081	77.517	1.00	14.67	C
ATOM	974	C	LYS	G	282	41.472	-21.113	78.988	1.00	11.17	C
ATOM	975	O	LYS	G	282	42.295	-21.293	79.875	1.00	8.39	O
ATOM	976	CB	LYS	G	282	42.063	-22.499	76.973	1.00	17.48	C
ATOM	977	CG	LYS	G	282	42.154	-22.568	75.439	1.00	21.17	C
ATOM	978	CD	LYS	G	282	42.219	-24.024	74.973	1.00	24.20	C
ATOM	979	CE	LYS	G	282	42.395	-24.173	73.455	1.00	23.38	C
ATOM	980	NZ	LYS	G	282	43.820	-24.133	72.979	1.00	20.23	N
ATOM	981	N	THR	G	283	40.177	-20.940	79.223	1.00	11.06	N
ATOM	982	CA	THR	G	283	39.601	-20.935	80.561	1.00	10.51	C
ATOM	983	C	THR	G	283	39.925	-22.237	81.297	1.00	11.20	C
ATOM	984	O	THR	G	283	40.004	-23.309	80.692	1.00	12.03	O
ATOM	985	CB	THR	G	283	38.049	-20.741	80.486	1.00	10.15	C
ATOM	986	OG1	THR	G	283	37.750	-19.505	79.819	1.00	10.23	O
ATOM	987	CG2	THR	G	283	37.419	-20.721	81.888	1.00	9.53	C
ATOM	988	N	ILE	G	284	40.163	-22.119	82.595	1.00	11.90	N
ATOM	989	CA	ILE	G	284	40.464	-23.263	83.449	1.00	11.48	C
ATOM	990	C	ILE	G	284	39.347	-23.214	84.472	1.00	10.31	C
ATOM	991	O	ILE	G	284	39.146	-22.186	85.112	1.00	9.75	O
ATOM	992	CB	ILE	G	284	41.836	-23.096	84.173	1.00	11.66	C
ATOM	993	CG1	ILE	G	284	42.954	-22.932	83.146	1.00	11.57	C
ATOM	994	CG2	ILE	G	284	42.148	-24.313	85.042	1.00	10.67	C
ATOM	995	CD1	ILE	G	284	44.301	-22.643	83.766	1.00	11.86	C
ATOM	996	N	ILE	G	285	38.547	-24.269	84.535	1.00	10.47	N
ATOM	997	CA	ILE	G	285	37.439	-24.326	85.480	1.00	9.39	C
ATOM	998	C	ILE	G	285	37.945	-25.046	86.718	1.00	10.51	C
ATOM	999	O	ILE	G	285	38.764	-25.961	86.614	1.00	12.99	O
ATOM	1000	CB	ILE	G	285	36.221	-25.084	84.892	1.00	8.03	C
ATOM	1001	CG1	ILE	G	285	35.891	-24.542	83.499	1.00	6.86	C
ATOM	1002	CG2	ILE	G	285	35.002	-24.894	85.785	1.00	7.78	C
ATOM	1003	CD1	ILE	G	285	34.648	-25.135	82.869	1.00	6.29	C
ATOM	1004	N	VAL	G	286	37.466	-24.636	87.886	1.00	9.48	N
ATOM	1005	CA	VAL	G	286	37.891	-25.237	89.140	1.00	6.38	C
ATOM	1006	C	VAL	G	286	36.680	-25.691	89.931	1.00	6.91	C
ATOM	1007	O	VAL	G	286	35.757	-24.914	90.182	1.00	6.45	O
ATOM	1008	CB	VAL	G	286	38.693	-24.218	90.006	1.00	6.91	C
ATOM	1009	CG1	VAL	G	286	39.106	-24.842	91.336	1.00	3.92	C
ATOM	1010	CG2	VAL	G	286	39.914	-23.692	89.239	1.00	2.85	C
ATOM	1011	N	GLN	G	287	36.679	-26.962	90.307	1.00	7.38	N
ATOM	1012	CA	GLN	G	287	35.597	-27.526	91.089	1.00	8.03	C
ATOM	1013	C	GLN	G	287	36.155	-27.618	92.489	1.00	10.75	C
ATOM	1014	O	GLN	G	287	37.217	-28.224	92.719	1.00	11.57	O
ATOM	1015	CB	GLN	G	287	35.194	-28.904	90.581	1.00	6.90	C
ATOM	1016	CG	GLN	G	287	34.006	-29.480	91.322	1.00	6.23	C
ATOM	1017	CD	GLN	G	287	33.402	-30.680	90.630	1.00	5.11	C
ATOM	1018	OE1	GLN	G	287	32.215	-30.695	90.337	1.00	7.55	O
ATOM	1019	NE2	GLN	G	287	34.216	-31.688	90.358	1.00	4.45	N
ATOM	1020	N	LEU	G	288	35.457	-26.980	93.419	1.00	12.14	N
ATOM	1021	CA	LEU	G	288	35.897	-26.930	94.797	1.00	13.73	C
ATOM	1022	C	LEU	G	288	35.544	-28.111	95.679	1.00	16.56	C
ATOM	1023	O	LEU	G	288	34.570	-28.830	95.440	1.00	18.23	O
ATOM	1024	CB	LEU	G	288	35.395	-25.644	95.440	1.00	12.23	C
ATOM	1025	CG	LEU	G	288	36.070	-24.354	94.998	1.00	8.03	C
ATOM	1026	CD1	LEU	G	288	35.785	-23.327	96.069	1.00	6.97	C
ATOM	1027	CD2	LEU	G	288	37.572	-24.551	94.868	1.00	5.62	C

FIG. 53-23

ATOM	1029	CA	ASN	G	289	36.137	-29.343	97.697	1.00	22.89	C
ATOM	1030	C	ASN	G	289	34.975	-29.000	98.617	1.00	24.07	C
ATOM	1031	O	ASN	G	289	34.020	-29.768	98.749	1.00	24.32	O
ATOM	1032	CB	ASN	G	289	37.390	-29.488	98.558	1.00	25.83	C
ATOM	1033	CG	ASN	G	289	38.022	-30.841	98.432	1.00	29.22	C
ATOM	1034	OD1	ASN	G	289	37.414	-31.762	97.894	1.00	30.49	O
ATOM	1035	ND2	ASN	G	289	39.277	-30.942	98.875	1.00	32.39	N
ATOM	1036	N	THR	G	290	35.064	-27.825	99.238	1.00	24.60	N
ATOM	1037	CA	THR	G	290	34.057	-27.352	100.182	1.00	24.63	C
ATOM	1038	C	THR	G	290	33.472	-26.014	99.721	1.00	23.12	C
ATOM	1039	O	THR	G	290	34.164	-25.199	99.108	1.00	22.54	O
ATOM	1040	CB	THR	G	290	34.688	-27.160	101.596	1.00	27.09	C
ATOM	1041	OG1	THR	G	290	35.516	-28.287	101.916	1.00	28.17	O
ATOM	1042	CG2	THR	G	290	33.600	-27.015	102.673	1.00	28.86	C
ATOM	1043	N	SER	G	291	32.191	-25.805	100.011	1.00	22.35	N
ATOM	1044	CA	SER	G	291	31.514	-24.564	99.655	1.00	21.82	C
ATOM	1045	C	SER	G	291	32.006	-23.411	100.523	1.00	22.98	C
ATOM	1046	O	SER	G	291	32.458	-23.603	101.661	1.00	22.87	O
ATOM	1047	CB	SER	G	291	29.998	-24.697	99.825	1.00	20.36	C
ATOM	1048	OG	SER	G	291	29.433	-25.549	98.847	1.00	19.98	O
ATOM	1049	N	VAL	G	292	31.919	-22.212	99.965	1.00	23.56	N
ATOM	1050	CA	VAL	G	292	32.323	-20.998	100.648	1.00	23.95	C
ATOM	1051	C	VAL	G	292	31.083	-20.136	100.522	1.00	24.36	C
ATOM	1052	O	VAL	G	292	30.268	-20.344	99.627	1.00	24.28	O
ATOM	1053	CB	VAL	G	292	33.497	-20.292	99.940	1.00	24.28	C
ATOM	1054	CG1	VAL	G	292	34.110	-19.254	100.862	1.00	24.70	C
ATOM	1055	CG2	VAL	G	292	34.539	-21.297	99.484	1.00	24.60	C
ATOM	1056	N	GLU	G	293	30.918	-19.185	101.424	1.00	24.79	N
ATOM	1057	CA	GLU	G	293	29.746	-18.335	101.378	1.00	25.81	C
ATOM	1058	C	GLU	G	293	30.106	-16.917	101.012	1.00	24.98	C
ATOM	1059	O	GLU	G	293	31.195	-16.426	101.335	1.00	26.72	O
ATOM	1060	CB	GLU	G	293	29.007	-18.372	102.718	1.00	26.15	C
ATOM	1061	CG	GLU	G	293	28.460	-19.745	103.042	1.00	27.81	C
ATOM	1062	CD	GLU	G	293	28.252	-19.948	104.512	1.00	29.06	C
ATOM	1063	OE1	GLU	G	293	29.244	-19.838	105.263	1.00	30.50	O
ATOM	1064	OE2	GLU	G	293	27.105	-20.234	104.920	1.00	31.07	O
ATOM	1065	N	ILE	G	294	29.193	-16.292	100.291	1.00	22.44	N
ATOM	1066	CA	ILE	G	294	29.343	-14.925	99.864	1.00	21.47	C
ATOM	1067	C	ILE	G	294	27.973	-14.292	100.076	1.00	22.05	C
ATOM	1068	O	ILE	G	294	26.999	-14.619	99.382	1.00	20.65	O
ATOM	1069	CB	ILE	G	294	29.841	-14.830	98.393	1.00	19.43	C
ATOM	1070	CG1	ILE	G	294	29.820	-13.382	97.910	1.00	14.54	C
ATOM	1071	CG2	ILE	G	294	29.041	-15.747	97.480	1.00	21.41	C
ATOM	1072	CD1	ILE	G	294	30.557	-13.184	96.630	1.00	7.75	C
ATOM	1073	N	ASN	G	295	27.890	-13.500	101.140	1.00	22.66	N
ATOM	1074	CA	ASN	G	295	26.663	-12.806	101.512	1.00	23.48	C
ATOM	1075	C	ASN	G	295	26.760	-11.408	100.912	1.00	22.67	C
ATOM	1076	O	ASN	G	295	27.787	-10.733	101.048	1.00	21.79	O
ATOM	1077	CB	ASN	G	295	26.526	-12.744	103.044	1.00	26.38	C
ATOM	1078	CG	ASN	G	295	26.744	-14.104	103.712	1.00	30.07	C
ATOM	1079	OD1	ASN	G	295	27.501	-14.929	103.197	1.00	31.57	O
ATOM	1080	ND2	ASN	G	295	26.102	-14.347	104.854	1.00	32.72	N
ATOM	1081	N	CYS	G	296	25.711	-10.999	100.205	1.00	23.39	N
ATOM	1082	CA	CYS	G	296	25.680	-9.693	99.555	1.00	23.29	C
ATOM	1083	C	CYS	G	296	24.345	-8.990	99.773	1.00	22.56	C
ATOM	1084	O	CYS	G	296	23.324	-9.641	100.001	1.00	20.72	O
ATOM	1085	CB	CYS	G	296	25.890	-9.853	98.049	1.00	24.78	C
ATOM	1086	SG	CYS	G	296	27.397	-10.728	97.530	1.00	27.71	S
ATOM	1087	N	THR	G	297	24.367	-7.665	99.647	1.00	22.54	N
ATOM	1088	CA	THR	G	297	23.188	-6.819	99.791	1.00	23.05	C
ATOM	1089	C	THR	G	297	23.247	-5.695	98.767	1.00	22.63	C
ATOM	1090	O	THR	G	297	24.331	-5.333	98.301	1.00	22.80	O
ATOM	1091	CB	THR	G	297	23.123	-6.169	101.178	1.00	24.92	C
ATOM	1092	OG1	THR	G	297	24.453	-5.961	101.665	1.00	27.02	O
ATOM	1093	CG2	THR	G	297	22.336	-7.023	102.147	1.00	25.66	C
ATOM	1094	N	GLY	G	298	22.091	-5.109	98.461	1.00	22.54	N
ATOM	1095	CA	GLY	G	298	22.029	-4.012	97.504	1.00	22.48	C
ATOM	1096	C	GLY	G	298	22.834	-2.795	97.940	1.00	21.63	C
ATOM	1097	O	GLY	G	298	23.237	-1.978	97.110	1.00	22.39	O
ATOM	1098	N	ALA	G	299	23.107	-2.716	99.242	1.00	20.04	N

FIG. 53-24

ATOM	1100	C	ALA	G	299	25.329	-1.540	99.408	1.00	18.55	C
ATOM	1101	O	ALA	G	299	26.147	-0.898	100.061	1.00	17.42	O
ATOM	1102	CB	ALA	G	299	23.822	-1.781	101.381	1.00	18.00	C
ATOM	1103	N	GLY	G	329	25.671	-2.248	98.340	1.00	20.79	N
ATOM	1104	CA	GLY	G	329	27.013	-2.165	97.804	1.00	21.75	C
ATOM	1105	C	GLY	G	329	28.117	-3.093	98.261	1.00	21.66	C
ATOM	1106	O	GLY	G	329	29.258	-2.900	97.858	1.00	21.50	O
ATOM	1107	N	HIS	G	330	27.835	-4.105	99.070	1.00	22.43	N
ATOM	1108	CA	HIS	G	330	28.926	-4.983	99.481	1.00	22.31	C
ATOM	1109	C	HIS	G	330	28.617	-6.461	99.535	1.00	21.45	C
ATOM	1110	O	HIS	G	330	27.458	-6.883	99.533	1.00	19.33	O
ATOM	1111	CB	HIS	G	330	29.563	-4.532	100.801	1.00	23.24	C
ATOM	1112	CG	HIS	G	330	28.574	-4.278	101.892	1.00	27.00	C
ATOM	1113	ND1	HIS	G	330	27.850	-5.258	102.527	1.00	27.17	N
ATOM	1114	CD2	HIS	G	330	28.168	-3.105	102.443	1.00	28.95	C
ATOM	1115	CE1	HIS	G	330	27.044	-4.667	103.417	1.00	28.28	C
ATOM	1116	NE2	HIS	G	330	27.204	-3.360	103.401	1.00	29.66	N
ATOM	1117	N	CYS	G	331	29.696	-7.233	99.510	1.00	22.55	N
ATOM	1118	CA	CYS	G	331	29.657	-8.682	99.575	1.00	24.15	C
ATOM	1119	C	CYS	G	331	30.739	-9.099	100.541	1.00	24.13	C
ATOM	1120	O	CYS	G	331	31.898	-8.726	100.370	1.00	24.27	O
ATOM	1121	CB	CYS	G	331	29.986	-9.299	98.220	1.00	24.97	C
ATOM	1122	SG	CYS	G	331	28.657	-9.223	97.000	1.00	28.48	S
ATOM	1123	N	ASN	G	332	30.382	-9.822	101.588	1.00	24.96	N
ATOM	1124	CA	ASN	G	332	31.425	-10.249	102.490	1.00	26.49	C
ATOM	1125	C	ASN	G	332	31.491	-11.767	102.519	1.00	24.08	C
ATOM	1126	O	ASN	G	332	30.474	-12.459	102.448	1.00	21.19	O
ATOM	1127	CB	ASN	G	332	31.289	-9.616	103.885	1.00	31.67	C
ATOM	1128	CG	ASN	G	332	30.507	-10.472	104.852	1.00	38.18	C
ATOM	1129	OD1	ASN	G	332	31.086	-11.014	105.792	1.00	41.31	O
ATOM	1130	ND2	ASN	G	332	29.213	-10.640	104.604	1.00	41.97	N
ATOM	1131	N	ILE	G	333	32.716	-12.258	102.470	1.00	23.04	N
ATOM	1132	CA	ILE	G	333	33.005	-13.677	102.489	1.00	23.16	C
ATOM	1133	C	ILE	G	333	34.098	-13.916	103.544	1.00	23.36	C
ATOM	1134	O	ILE	G	333	35.029	-13.109	103.685	1.00	21.86	O
ATOM	1135	CB	ILE	G	333	33.422	-14.178	101.062	1.00	21.56	C
ATOM	1136	CG1	ILE	G	333	34.577	-15.170	101.137	1.00	19.40	C
ATOM	1137	CG2	ILE	G	333	33.748	-12.997	100.141	1.00	22.44	C
ATOM	1138	CD1	ILE	G	333	35.100	-15.539	99.807	1.00	17.23	C
ATOM	1139	N	SER	G	334	33.953	-14.992	104.315	1.00	22.28	N
ATOM	1140	CA	SER	G	334	34.917	-15.324	105.355	1.00	22.05	C
ATOM	1141	C	SER	G	334	36.355	-15.342	104.839	1.00	22.63	C
ATOM	1142	O	SER	G	334	36.673	-15.995	103.847	1.00	22.64	O
ATOM	1143	CB	SER	G	334	34.560	-16.662	105.997	1.00	22.04	C
ATOM	1144	OG	SER	G	334	33.172	-16.722	106.305	1.00	22.98	O
ATOM	1145	N	ARG	G	335	37.207	-14.589	105.516	1.00	24.33	N
ATOM	1146	CA	ARG	G	335	38.617	-14.473	105.174	1.00	26.14	C
ATOM	1147	C	ARG	G	335	39.384	-15.794	105.297	1.00	26.30	C
ATOM	1148	O	ARG	G	335	40.233	-16.103	104.464	1.00	26.93	O
ATOM	1149	CB	ARG	G	335	39.246	-13.419	106.085	1.00	28.38	C
ATOM	1150	CG	ARG	G	335	40.747	-13.345	106.044	1.00	32.38	C
ATOM	1151	CD	ARG	G	335	41.256	-12.299	107.027	1.00	39.28	C
ATOM	1152	NE	ARG	G	335	40.577	-11.012	106.869	1.00	44.47	N
ATOM	1153	CZ	ARG	G	335	40.903	-9.902	107.526	1.00	48.65	C
ATOM	1154	NH1	ARG	G	335	41.915	-9.906	108.386	1.00	50.25	N
ATOM	1155	NH2	ARG	G	335	40.184	-8.799	107.363	1.00	50.93	N
ATOM	1156	N	ALA	G	336	39.105	-16.549	106.358	1.00	25.12	N
ATOM	1157	CA	ALA	G	336	39.777	-17.820	106.603	1.00	23.00	C
ATOM	1158	C	ALA	G	336	39.305	-18.899	105.634	1.00	22.42	C
ATOM	1159	O	ALA	G	336	40.128	-19.554	104.981	1.00	21.64	O
ATOM	1160	CB	ALA	G	336	39.563	-18.259	108.034	1.00	23.10	C
ATOM	1161	N	LYS	G	337	37.985	-19.048	105.507	1.00	21.05	N
ATOM	1162	CA	LYS	G	337	37.405	-20.040	104.608	1.00	20.30	C
ATOM	1163	C	LYS	G	337	37.964	-19.926	103.202	1.00	20.37	C
ATOM	1164	O	LYS	G	337	38.345	-20.926	102.597	1.00	20.21	O
ATOM	1165	CB	LYS	G	337	35.886	-19.907	104.540	1.00	20.28	C
ATOM	1166	CG	LYS	G	337	35.121	-20.622	105.642	1.00	22.99	C
ATOM	1167	CD	LYS	G	337	33.606	-20.410	105.465	1.00	25.82	C
ATOM	1168	CE	LYS	G	337	32.784	-20.963	106.637	1.00	26.21	C
ATOM	1169	NZ	LYS	G	337	31.427	-20.343	106.712	1.00	27.47	N

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FIG. 53-25

ATOM	1171	CA	TRP	G	338	38.528	-18.528	101.324	1.00	21.84	C
ATOM	1172	C	TRP	G	338	40.036	-18.605	101.126	1.00	22.14	C
ATOM	1173	O	TRP	G	338	40.498	-18.997	100.050	1.00	21.87	O
ATOM	1174	CB	TRP	G	338	37.983	-17.238	100.704	1.00	20.93	C
ATOM	1175	CG	TRP	G	338	37.657	-17.425	99.263	1.00	20.83	C
ATOM	1176	CD1	TRP	G	338	36.578	-18.083	98.743	1.00	22.75	C
ATOM	1177	CD2	TRP	G	338	38.426	-16.979	98.144	1.00	19.66	C
ATOM	1178	NE1	TRP	G	338	36.627	-18.071	97.368	1.00	22.40	N
ATOM	1179	CE2	TRP	G	338	37.753	-17.403	96.975	1.00	19.83	C
ATOM	1180	CE3	TRP	G	338	39.618	-16.261	98.012	1.00	19.32	C
ATOM	1181	CZ2	TRP	G	338	38.231	-17.134	95.696	1.00	21.02	C
ATOM	1182	CZ3	TRP	G	338	40.091	-15.997	96.743	1.00	21.47	C
ATOM	1183	CH2	TRP	G	338	39.400	-16.432	95.599	1.00	21.53	C
ATOM	1184	N	ASN	G	339	40.812	-18.216	102.132	1.00	22.61	N
ATOM	1185	CA	ASN	G	339	42.256	-18.276	101.969	1.00	25.09	C
ATOM	1186	C	ASN	G	339	42.681	-19.747	101.917	1.00	24.55	C
ATOM	1187	O	ASN	G	339	43.653	-20.109	101.250	1.00	23.39	O
ATOM	1188	CB	ASN	G	339	42.972	-17.521	103.090	1.00	29.69	C
ATOM	1189	CG	ASN	G	339	44.411	-17.175	102.733	1.00	37.25	C
ATOM	1190	OD1	ASN	G	339	45.358	-17.669	103.354	1.00	38.36	O
ATOM	1191	ND2	ASN	G	339	44.579	-16.334	101.712	1.00	44.12	N
ATOM	1192	N	ASN	G	340	41.898	-20.597	102.574	1.00	24.15	N
ATOM	1193	CA	ASN	G	340	42.162	-22.028	102.602	1.00	24.49	C
ATOM	1194	C	ASN	G	340	41.929	-22.666	101.228	1.00	22.71	C
ATOM	1195	O	ASN	G	340	42.763	-23.431	100.742	1.00	22.28	O
ATOM	1196	CB	ASN	G	340	41.285	-22.715	103.652	1.00	28.25	C
ATOM	1197	CG	ASN	G	340	41.691	-24.158	103.901	1.00	32.25	C
ATOM	1198	OD1	ASN	G	340	41.044	-25.090	103.421	1.00	34.35	O
ATOM	1199	ND2	ASN	G	340	42.776	-24.348	104.646	1.00	32.79	N
ATOM	1200	N	THR	G	341	40.804	-22.344	100.595	1.00	20.42	N
ATOM	1201	CA	THR	G	341	40.498	-22.898	99.275	1.00	18.47	C
ATOM	1202	C	THR	G	341	41.539	-22.452	98.256	1.00	16.79	C
ATOM	1203	O	THR	G	341	41.774	-23.132	97.253	1.00	16.74	O
ATOM	1204	CB	THR	G	341	39.106	-22.458	98.758	1.00	18.47	C
ATOM	1205	OG1	THR	G	341	39.154	-21.093	98.322	1.00	15.57	O
ATOM	1206	CG2	THR	G	341	38.063	-22.601	99.857	1.00	17.91	C
ATOM	1207	N	LEU	G	342	42.160	-21.306	98.515	1.00	15.68	N
ATOM	1208	CA	LEU	G	342	43.162	-20.765	97.614	1.00	15.72	C
ATOM	1209	C	LEU	G	342	44.400	-21.624	97.584	1.00	15.53	C
ATOM	1210	O	LEU	G	342	44.904	-21.940	96.510	1.00	15.44	O
ATOM	1211	CB	LEU	G	342	43.521	-19.332	98.000	1.00	18.54	C
ATOM	1212	CG	LEU	G	342	42.615	-18.175	97.567	1.00	18.13	C
ATOM	1213	CD1	LEU	G	342	42.933	-16.964	98.423	1.00	15.23	C
ATOM	1214	CD2	LEU	G	342	42.794	-17.866	96.079	1.00	14.33	C
ATOM	1215	N	LYS	G	343	44.882	-22.027	98.758	1.00	16.83	N
ATOM	1216	CA	LYS	G	343	46.077	-22.869	98.825	1.00	17.44	C
ATOM	1217	C	LYS	G	343	45.775	-24.266	98.306	1.00	18.33	C
ATOM	1218	O	LYS	G	343	46.680	-24.992	97.920	1.00	19.02	O
ATOM	1219	CB	LYS	G	343	46.672	-22.924	100.238	1.00	15.61	C
ATOM	1220	CG	LYS	G	343	45.875	-23.699	101.266	1.00	17.55	C
ATOM	1221	CD	LYS	G	343	46.755	-24.097	102.450	1.00	19.36	C
ATOM	1222	CE	LYS	G	343	47.847	-25.094	102.038	1.00	22.94	C
ATOM	1223	NZ	LYS	G	343	47.289	-26.365	101.448	1.00	25.97	N
ATOM	1224	N	GLN	G	344	44.503	-24.651	98.334	1.00	19.88	N
ATOM	1225	CA	GLN	G	344	44.084	-25.948	97.820	1.00	22.64	C
ATOM	1226	C	GLN	G	344	44.181	-25.876	96.294	1.00	24.58	C
ATOM	1227	O	GLN	G	344	44.821	-26.719	95.661	1.00	27.10	O
ATOM	1228	CB	GLN	G	344	42.648	-26.269	98.237	1.00	22.13	C
ATOM	1229	CG	GLN	G	344	42.470	-26.496	99.728	1.00	23.77	C
ATOM	1230	CD	GLN	G	344	41.046	-26.867	100.099	1.00	25.77	C
ATOM	1231	OE1	GLN	G	344	40.126	-26.805	99.270	1.00	29.28	O
ATOM	1232	NE2	GLN	G	344	40.853	-27.257	101.349	1.00	25.33	N
ATOM	1233	N	ILE	G	345	43.565	-24.849	95.713	1.00	24.68	N
ATOM	1234	CA	ILE	G	345	43.601	-24.645	94.274	1.00	23.26	C
ATOM	1235	C	ILE	G	345	45.057	-24.451	93.871	1.00	22.65	C
ATOM	1236	O	ILE	G	345	45.463	-24.877	92.791	1.00	24.30	O
ATOM	1237	CB	ILE	G	345	42.803	-23.386	93.861	1.00	24.27	C
ATOM	1238	CG1	ILE	G	345	41.344	-23.508	94.325	1.00	23.39	C
ATOM	1239	CG2	ILE	G	345	42.894	-23.172	92.347	1.00	22.15	C
ATOM	1240	CD1	ILE	G	345	40.500	-22.272	94.070	1.00	20.49	C

FIG. 53-26

ATOM	1242	CA	ALA	G	346	47.261	-23.598	94.462	1.00	19.48	C
ATOM	1243	C	ALA	G	346	48.045	-24.906	94.412	1.00	20.48	C
ATOM	1244	O	ALA	G	346	49.036	-25.020	93.697	1.00	20.51	O
ATOM	1245	CB	ALA	G	346	47.859	-22.658	95.501	1.00	17.62	C
ATOM	1246	N	SER	G	347	47.553	-25.911	95.126	1.00	22.28	N
ATOM	1247	CA	SER	G	347	48.199	-27.212	95.169	1.00	24.38	C
ATOM	1248	C	SER	G	347	47.989	-28.031	93.901	1.00	26.23	C
ATOM	1249	O	SER	G	347	47.940	-29.261	93.966	1.00	26.76	O
ATOM	1250	CB	SER	G	347	47.699	-28.008	96.375	1.00	24.17	C
ATOM	1251	OG	SER	G	347	48.063	-27.385	97.598	1.00	24.21	O
ATOM	1252	N	LYS	G	348	47.839	-27.364	92.757	1.00	29.96	N
ATOM	1253	CA	LYS	G	348	47.642	-28.065	91.489	1.00	33.03	C
ATOM	1254	C	LYS	G	348	47.559	-27.230	90.221	1.00	35.63	C
ATOM	1255	O	LYS	G	348	47.321	-27.788	89.152	1.00	38.39	O
ATOM	1256	CB	LYS	G	348	46.413	-28.975	91.565	1.00	32.95	C
ATOM	1257	CG	LYS	G	348	45.129	-28.281	91.999	1.00	33.51	C
ATOM	1258	CD	LYS	G	348	44.028	-29.304	92.276	1.00	31.97	C
ATOM	1259	CE	LYS	G	348	43.720	-30.135	91.034	1.00	30.77	C
ATOM	1260	NZ	LYS	G	348	43.968	-31.571	91.245	1.00	29.18	N
ATOM	1261	N	LEU	G	349	47.844	-25.935	90.296	1.00	37.19	N
ATOM	1262	CA	LEU	G	349	47.740	-25.060	89.121	1.00	39.86	C
ATOM	1263	C	LEU	G	349	48.595	-25.380	87.879	1.00	40.94	C
ATOM	1264	O	LEU	G	349	49.636	-26.019	87.995	1.00	40.31	O
ATOM	1265	CB	LEU	G	349	47.868	-23.602	89.553	1.00	39.82	C
ATOM	1266	CG	LEU	G	349	46.582	-23.193	90.277	1.00	39.38	C
ATOM	1267	CD1	LEU	G	349	46.704	-21.816	90.896	1.00	38.81	C
ATOM	1268	CD2	LEU	G	349	45.419	-23.268	89.287	1.00	38.70	C
ATOM	1269	N	ARG	G	350	48.123	-24.926	86.708	1.00	42.25	N
ATOM	1270	CA	ARG	G	350	48.719	-25.151	85.371	1.00	42.80	C
ATOM	1271	C	ARG	G	350	49.867	-26.116	85.187	1.00	43.82	C
ATOM	1272	O	ARG	G	350	49.823	-26.941	84.275	1.00	45.61	O
ATOM	1273	CB	ARG	G	350	49.039	-23.866	84.619	1.00	43.22	C
ATOM	1274	CG	ARG	G	350	49.218	-24.105	83.101	1.00	45.68	C
ATOM	1275	CD	ARG	G	350	50.614	-24.613	82.682	1.00	49.73	C
ATOM	1276	NE	ARG	G	350	50.589	-25.386	81.431	1.00	52.41	N
ATOM	1277	CZ	ARG	G	350	51.606	-26.114	80.961	1.00	51.60	C
ATOM	1278	NH1	ARG	G	350	52.750	-26.185	81.632	1.00	53.56	N
ATOM	1279	NH2	ARG	G	350	51.476	-26.793	79.831	1.00	51.64	N
ATOM	1280	N	GLU	G	351	50.932	-25.965	85.967	1.00	43.58	N
ATOM	1281	CA	GLU	G	351	52.082	-26.872	85.906	1.00	43.20	C
ATOM	1282	C	GLU	G	351	51.500	-28.298	85.840	1.00	43.33	C
ATOM	1283	O	GLU	G	351	52.113	-29.209	85.285	1.00	42.89	O
ATOM	1284	CB	GLU	G	351	52.924	-26.670	87.174	1.00	43.52	C
ATOM	1285	CG	GLU	G	351	54.310	-27.289	87.200	1.00	41.21	C
ATOM	1286	CD	GLU	G	351	55.019	-27.057	88.534	1.00	41.51	C
ATOM	1287	OE1	GLU	G	351	54.342	-26.751	89.541	1.00	40.87	O
ATOM	1288	OE2	GLU	G	351	56.259	-27.169	88.583	1.00	42.54	O
ATOM	1289	N	GLN	G	352	50.280	-28.429	86.375	1.00	43.75	N
ATOM	1290	CA	GLN	G	352	49.473	-29.647	86.408	1.00	45.18	C
ATOM	1291	C	GLN	G	352	49.718	-30.460	87.656	1.00	46.24	C
ATOM	1292	O	GLN	G	352	50.300	-31.549	87.611	1.00	46.13	O
ATOM	1293	CB	GLN	G	352	49.649	-30.483	85.132	1.00	45.24	C
ATOM	1294	CG	GLN	G	352	48.880	-29.946	83.930	1.00	43.09	C
ATOM	1295	CD	GLN	G	352	47.404	-29.785	84.226	1.00	42.64	C
ATOM	1296	OE1	GLN	G	352	46.589	-30.619	83.838	1.00	42.75	O
ATOM	1297	NE2	GLN	G	352	47.051	-28.708	84.922	1.00	41.31	N
ATOM	1298	N	PHE	G	353	49.221	-29.927	88.770	1.00	47.62	N
ATOM	1299	CA	PHE	G	353	49.396	-30.535	90.086	1.00	49.37	C
ATOM	1300	C	PHE	G	353	50.909	-30.583	90.244	1.00	50.92	C
ATOM	1301	O	PHE	G	353	51.465	-31.458	90.910	1.00	51.55	O
ATOM	1302	CB	PHE	G	353	48.784	-31.939	90.124	1.00	48.39	C
ATOM	1303	CG	PHE	G	353	48.379	-32.391	91.499	1.00	47.75	C
ATOM	1304	CD1	PHE	G	353	49.304	-32.437	92.536	1.00	47.81	C
ATOM	1305	CD2	PHE	G	353	47.071	-32.794	91.750	1.00	47.05	C
ATOM	1306	CE1	PHE	G	353	48.936	-32.876	93.804	1.00	48.78	C
ATOM	1307	CE2	PHE	G	353	46.691	-33.234	93.013	1.00	47.45	C
ATOM	1308	CZ	PHE	G	353	47.625	-33.276	94.042	1.00	48.43	C
ATOM	1309	N	GLY	G	354	51.556	-29.613	89.602	1.00	52.21	N
ATOM	1310	CA	GLY	G	354	52.996	-29.519	89.600	1.00	55.31	C
ATOM	1311	C	GLY	G	354	53.623	-29.810	90.936	1.00	57.09	C

FIG. 53-27

ATOM	1313	N	ASN	G	355	54.716	-30.563	90.895	1.00	56.63	N
ATOM	1314	CA	ASN	G	355	55.437	-30.927	92.100	1.00	55.92	C
ATOM	1315	C	ASN	G	355	55.702	-29.673	92.922	1.00	54.78	C
ATOM	1316	O	ASN	G	355	55.635	-29.727	94.155	1.00	55.56	O
ATOM	1317	CB	ASN	G	355	56.729	-31.658	91.742	1.00	56.52	C
ATOM	1318	CG	ASN	G	355	56.474	-32.950	90.982	1.00	57.60	C
ATOM	1319	OD1	ASN	G	355	57.404	-33.565	90.467	1.00	60.33	O
ATOM	1320	ND2	ASN	G	355	55.212	-33.359	90.895	1.00	56.65	N
ATOM	1321	N	ASN	G	356	55.994	-28.560	92.238	1.00	51.48	N
ATOM	1322	CA	ASN	G	356	56.209	-27.270	92.891	1.00	48.76	C
ATOM	1323	C	ASN	G	356	56.815	-26.133	92.083	1.00	47.04	C
ATOM	1324	O	ASN	G	356	57.690	-26.330	91.233	1.00	46.83	O
ATOM	1325	CB	ASN	G	356	56.969	-27.398	94.205	1.00	49.07	C
ATOM	1326	CG	ASN	G	356	56.270	-26.671	95.331	1.00	50.28	C
ATOM	1327	OD1	ASN	G	356	55.666	-25.613	95.121	1.00	49.32	O
ATOM	1328	ND2	ASN	G	356	56.322	-27.241	96.528	1.00	50.39	N
ATOM	1329	N	LYS	G	357	56.344	-24.932	92.417	1.00	44.39	N
ATOM	1330	CA	LYS	G	357	56.759	-23.666	91.824	1.00	41.03	C
ATOM	1331	C	LYS	G	357	55.913	-22.592	92.496	1.00	40.06	C
ATOM	1332	O	LYS	G	357	55.035	-22.899	93.307	1.00	40.50	O
ATOM	1333	CB	LYS	G	357	56.537	-23.631	90.316	1.00	39.41	C
ATOM	1334	CG	LYS	G	357	55.084	-23.571	89.867	1.00	37.01	C
ATOM	1335	CD	LYS	G	357	55.017	-23.221	88.392	1.00	35.55	C
ATOM	1336	CE	LYS	G	357	56.110	-23.954	87.642	1.00	33.79	C
ATOM	1337	NZ	LYS	G	357	56.188	-23.600	86.218	1.00	34.41	N
ATOM	1338	N	THR	G	358	56.160	-21.337	92.150	1.00	37.88	N
ATOM	1339	CA	THR	G	358	55.430	-20.231	92.746	1.00	35.21	C
ATOM	1340	C	THR	G	358	54.093	-20.001	92.042	1.00	32.30	C
ATOM	1341	O	THR	G	358	54.055	-19.800	90.826	1.00	32.63	O
ATOM	1342	CB	THR	G	358	56.270	-18.922	92.688	1.00	36.59	C
ATOM	1343	OG1	THR	G	358	57.648	-19.203	92.988	1.00	36.43	O
ATOM	1344	CG2	THR	G	358	55.738	-17.902	93.691	1.00	36.20	C
ATOM	1345	N	ILE	G	359	53.002	-20.066	92.798	1.00	28.71	N
ATOM	1346	CA	ILE	G	359	51.667	-19.833	92.255	1.00	25.73	C
ATOM	1347	C	ILE	G	359	51.187	-18.455	92.712	1.00	25.01	C
ATOM	1348	O	ILE	G	359	51.098	-18.175	93.910	1.00	25.59	O
ATOM	1349	CB	ILE	G	359	50.664	-20.923	92.700	1.00	25.07	C
ATOM	1350	CG1	ILE	G	359	50.695	-22.099	91.723	1.00	23.68	C
ATOM	1351	CG2	ILE	G	359	49.245	-20.367	92.786	1.00	24.79	C
ATOM	1352	CD1	ILE	G	359	51.903	-22.969	91.841	1.00	24.61	C
ATOM	1353	N	ILE	G	360	50.859	-17.599	91.755	1.00	23.10	N
ATOM	1354	CA	ILE	G	360	50.423	-16.252	92.074	1.00	20.52	C
ATOM	1355	C	ILE	G	360	49.004	-15.969	91.600	1.00	21.12	C
ATOM	1356	O	ILE	G	360	48.611	-16.308	90.477	1.00	19.68	O
ATOM	1357	CB	ILE	G	360	51.386	-15.193	91.474	1.00	18.01	C
ATOM	1358	CG1	ILE	G	360	52.818	-15.474	91.921	1.00	19.32	C
ATOM	1359	CG2	ILE	G	360	51.009	-13.806	91.945	1.00	16.83	C
ATOM	1360	CD1	ILE	G	360	53.863	-14.699	91.178	1.00	20.28	C
ATOM	1361	N	PHE	G	361	48.232	-15.375	92.498	1.00	21.60	N
ATOM	1362	CA	PHE	G	361	46.867	-14.990	92.223	1.00	20.51	C
ATOM	1363	C	PHE	G	361	46.838	-13.468	92.138	1.00	20.25	C
ATOM	1364	O	PHE	G	361	47.157	-12.789	93.115	1.00	20.96	O
ATOM	1365	CB	PHE	G	361	45.939	-15.457	93.348	1.00	18.51	C
ATOM	1366	CG	PHE	G	361	45.647	-16.935	93.330	1.00	19.11	C
ATOM	1367	CD1	PHE	G	361	45.126	-17.546	92.191	1.00	19.66	C
ATOM	1368	CD2	PHE	G	361	45.875	-17.718	94.458	1.00	17.60	C
ATOM	1369	CE1	PHE	G	361	44.840	-18.915	92.181	1.00	18.26	C
ATOM	1370	CE2	PHE	G	361	45.593	-19.080	94.450	1.00	16.64	C
ATOM	1371	CZ	PHE	G	361	45.075	-19.678	93.311	1.00	16.40	C
ATOM	1372	N	LYS	G	362	46.581	-12.951	90.940	1.00	19.16	N
ATOM	1373	CA	LYS	G	362	46.456	-11.512	90.707	1.00	17.16	C
ATOM	1374	C	LYS	G	362	45.026	-11.365	90.215	1.00	16.29	C
ATOM	1375	O	LYS	G	362	44.293	-12.353	90.132	1.00	16.31	O
ATOM	1376	CB	LYS	G	362	47.395	-11.011	89.603	1.00	16.96	C
ATOM	1377	CG	LYS	G	362	48.850	-10.842	89.992	1.00	17.71	C
ATOM	1378	CD	LYS	G	362	49.596	-10.118	88.874	1.00	18.34	C
ATOM	1379	CE	LYS	G	362	51.021	-10.631	88.709	1.00	17.10	C
ATOM	1380	NZ	LYS	G	362	51.864	-10.418	89.909	1.00	18.10	N
ATOM	1381	N	GLN	G	363	44.625	-10.149	89.861	1.00	15.68	N
ATOM	1382	CA	GLN	G	363	43.272	-9.948	89.377	1.00	15.22	C

FIG. 53-28

ATOM	1384	O	GLN	G	363	44.245	-9.483	87.236	1.00	13.77	O
ATOM	1385	CB	GLN	G	363	42.529	-8.939	90.231	1.00	19.40	C
ATOM	1386	CG	GLN	G	363	41.196	-9.469	90.728	1.00	24.43	C
ATOM	1387	CD	GLN	G	363	40.033	-8.844	90.008	1.00	27.66	C
ATOM	1388	OE1	GLN	G	363	39.942	-7.621	89.904	1.00	29.28	O
ATOM	1389	NE2	GLN	G	363	39.123	-9.671	89.518	1.00	29.73	N
ATOM	1390	N	SER	G	364	41.996	-9.403	87.413	1.00	12.57	N
ATOM	1391	CA	SER	G	364	41.775	-9.117	86.016	1.00	12.09	C
ATOM	1392	C	SER	G	364	42.651	-8.048	85.392	1.00	14.93	C
ATOM	1393	O	SER	G	364	42.913	-7.004	85.994	1.00	15.10	O
ATOM	1394	CB	SER	G	364	40.317	-8.783	85.783	1.00	11.50	C
ATOM	1395	OG	SER	G	364	40.006	-8.944	84.414	1.00	12.57	O
ATOM	1396	N	SER	G	365	43.107	-8.333	84.174	1.00	16.70	N
ATOM	1397	CA	SER	G	365	43.941	-7.409	83.412	1.00	15.93	C
ATOM	1398	C	SER	G	365	43.067	-6.254	82.898	1.00	14.17	C
ATOM	1399	O	SER	G	365	43.514	-5.103	82.821	1.00	12.17	O
ATOM	1400	CB	SER	G	365	44.572	-8.129	82.220	1.00	15.75	C
ATOM	1401	OG	SER	G	365	45.334	-9.256	82.612	1.00	17.45	O
ATOM	1402	N	GLY	G	366	41.835	-6.581	82.515	1.00	11.39	N
ATOM	1403	CA	GLY	G	366	40.931	-5.571	82.002	1.00	9.59	C
ATOM	1404	C	GLY	G	366	39.815	-6.159	81.165	1.00	7.26	C
ATOM	1405	O	GLY	G	366	39.727	-7.377	81.003	1.00	5.86	O
ATOM	1406	N	GLY	G	367	38.993	-5.286	80.594	1.00	6.94	N
ATOM	1407	CA	GLY	G	367	37.877	-5.730	79.779	1.00	6.56	C
ATOM	1408	C	GLY	G	367	36.551	-5.336	80.396	1.00	6.41	C
ATOM	1409	O	GLY	G	367	36.512	-4.652	81.419	1.00	4.55	O
ATOM	1410	N	ASP	G	368	35.463	-5.785	79.782	1.00	8.86	N
ATOM	1411	CA	ASP	G	368	34.111	-5.480	80.254	1.00	11.00	C
ATOM	1412	C	ASP	G	368	33.917	-5.533	81.767	1.00	12.56	C
ATOM	1413	O	ASP	G	368	34.601	-6.284	82.470	1.00	14.21	O
ATOM	1414	CB	ASP	G	368	33.118	-6.431	79.603	1.00	11.95	C
ATOM	1415	CG	ASP	G	368	32.804	-6.052	78.182	1.00	14.99	C
ATOM	1416	OD1	ASP	G	368	33.720	-5.637	77.432	1.00	15.86	O
ATOM	1417	OD2	ASP	G	368	31.627	-6.185	77.800	1.00	14.92	O
ATOM	1418	N	PRO	G	369	32.957	-4.750	82.292	1.00	12.32	N
ATOM	1419	CA	PRO	G	369	32.703	-4.741	83.726	1.00	11.90	C
ATOM	1420	C	PRO	G	369	32.277	-6.132	84.202	1.00	11.43	C
ATOM	1421	O	PRO	G	369	32.726	-6.598	85.239	1.00	11.49	O
ATOM	1422	CB	PRO	G	369	31.562	-3.730	83.852	1.00	12.76	C
ATOM	1423	CG	PRO	G	369	31.783	-2.809	82.728	1.00	10.24	C
ATOM	1424	CD	PRO	G	369	32.084	-3.773	81.622	1.00	13.28	C
ATOM	1425	N	GLU	G	370	31.450	-6.807	83.410	1.00	11.25	N
ATOM	1426	CA	GLU	G	370	30.954	-8.149	83.747	1.00	11.17	C
ATOM	1427	C	GLU	G	370	32.078	-9.175	83.855	1.00	9.72	C
ATOM	1428	O	GLU	G	370	31.950	-10.168	84.563	1.00	9.84	O
ATOM	1429	CB	GLU	G	370	29.939	-8.628	82.709	1.00	12.14	C
ATOM	1430	CG	GLU	G	370	28.763	-7.683	82.449	1.00	14.26	C
ATOM	1431	CD	GLU	G	370	29.133	-6.422	81.665	1.00	13.73	C
ATOM	1432	OE1	GLU	G	370	30.216	-6.377	81.046	1.00	15.24	O
ATOM	1433	OE2	GLU	G	370	28.335	-5.463	81.652	1.00	12.38	O
ATOM	1434	N	ILE	G	371	33.171	-8.919	83.141	1.00	8.48	N
ATOM	1435	CA	ILE	G	371	34.359	-9.777	83.114	1.00	6.27	C
ATOM	1436	C	ILE	G	371	35.372	-9.461	84.213	1.00	5.63	C
ATOM	1437	O	ILE	G	371	35.946	-10.375	84.819	1.00	3.51	O
ATOM	1438	CB	ILE	G	371	35.057	-9.664	81.726	1.00	7.86	C
ATOM	1439	CG1	ILE	G	371	34.249	-10.438	80.699	1.00	10.27	C
ATOM	1440	CG2	ILE	G	371	36.518	-10.107	81.770	1.00	5.95	C
ATOM	1441	CD1	ILE	G	371	33.646	-11.702	81.270	1.00	14.03	C
ATOM	1442	N	VAL	G	372	35.609	-8.163	84.420	1.00	5.08	N
ATOM	1443	CA	VAL	G	372	36.553	-7.638	85.406	1.00	5.14	C
ATOM	1444	C	VAL	G	372	36.064	-7.739	86.862	1.00	6.39	C
ATOM	1445	O	VAL	G	372	36.860	-7.658	87.808	1.00	4.88	O
ATOM	1446	CB	VAL	G	372	36.884	-6.163	85.084	1.00	4.04	C
ATOM	1447	CG1	VAL	G	372	37.827	-5.577	86.108	1.00	4.81	C
ATOM	1448	CG2	VAL	G	372	37.525	-6.075	83.734	1.00	5.30	C
ATOM	1449	N	THR	G	373	34.766	-7.939	87.046	1.00	7.07	N
ATOM	1450	CA	THR	G	373	34.200	-8.032	88.383	1.00	6.38	C
ATOM	1451	C	THR	G	373	33.254	-9.236	88.503	1.00	6.11	C
ATOM	1452	O	THR	G	373	32.762	-9.720	87.489	1.00	7.72	O
ATOM	1453	CB	THR	G	373	33.449	-6.717	88.726	1.00	3.53	C

FIG. 53-29

ATOM	1455	CG2	THR	G	373	34.341	-5.514	88.499	1.00	2.00	C
ATOM	1456	N	HIS	G	374	33.034	-9.737	89.721	1.00	5.67	N
ATOM	1457	CA	HIS	G	374	32.119	-10.868	89.931	1.00	7.82	C
ATOM	1458	C	HIS	G	374	30.696	-10.362	89.714	1.00	9.15	C
ATOM	1459	O	HIS	G	374	30.019	-9.989	90.667	1.00	10.34	O
ATOM	1460	CB	HIS	G	374	32.259	-11.466	91.362	1.00	5.94	C
ATOM	1461	CG	HIS	G	374	31.164	-12.434	91.746	1.00	6.61	C
ATOM	1462	ND1	HIS	G	374	30.810	-13.523	90.976	1.00	4.93	N
ATOM	1463	CD2	HIS	G	374	30.312	-12.444	92.803	1.00	6.52	C
ATOM	1464	CE1	HIS	G	374	29.786	-14.148	91.527	1.00	2.00	C
ATOM	1465	NE2	HIS	G	374	29.464	-13.516	92.641	1.00	2.00	N
ATOM	1466	N	SER	G	375	30.256	-10.317	88.462	1.00	10.09	N
ATOM	1467	CA	SER	G	375	28.906	-9.852	88.149	1.00	10.24	C
ATOM	1468	C	SER	G	375	27.942	-11.016	88.248	1.00	9.46	C
ATOM	1469	O	SER	G	375	28.258	-12.147	87.866	1.00	9.82	O
ATOM	1470	CB	SER	G	375	28.848	-9.240	86.749	1.00	11.18	C
ATOM	1471	OG	SER	G	375	29.837	-8.236	86.596	1.00	14.87	O
ATOM	1472	N	PHE	G	376	26.755	-10.739	88.752	1.00	8.32	N
ATOM	1473	CA	PHE	G	376	25.750	-11.767	88.920	1.00	8.62	C
ATOM	1474	C	PHE	G	376	24.419	-11.086	89.133	1.00	9.88	C
ATOM	1475	O	PHE	G	376	24.358	-9.868	89.298	1.00	9.95	O
ATOM	1476	CB	PHE	G	376	26.085	-12.633	90.144	1.00	8.97	C
ATOM	1477	CG	PHE	G	376	26.292	-11.848	91.412	1.00	6.84	C
ATOM	1478	CD1	PHE	G	376	27.530	-11.271	91.692	1.00	4.82	C
ATOM	1479	CD2	PHE	G	376	25.245	-11.662	92.314	1.00	5.82	C
ATOM	1480	CE1	PHE	G	376	27.727	-10.523	92.848	1.00	2.00	C
ATOM	1481	CE2	PHE	G	376	25.429	-10.918	93.470	1.00	3.10	C
ATOM	1482	CZ	PHE	G	376	26.674	-10.346	93.737	1.00	4.76	C
ATOM	1483	N	ASN	G	377	23.343	-11.857	89.097	1.00	12.53	N
ATOM	1484	CA	ASN	G	377	22.038	-11.266	89.317	1.00	15.48	C
ATOM	1485	C	ASN	G	377	21.530	-11.603	90.706	1.00	17.28	C
ATOM	1486	O	ASN	G	377	21.080	-12.717	90.963	1.00	18.65	O
ATOM	1487	CB	ASN	G	377	21.019	-11.710	88.272	1.00	13.51	C
ATOM	1488	CG	ASN	G	377	19.762	-10.887	88.331	1.00	11.15	C
ATOM	1489	OD1	ASN	G	377	18.847	-11.184	89.092	1.00	11.21	O
ATOM	1490	ND2	ASN	G	377	19.739	-9.803	87.578	1.00	10.80	N
ATOM	1491	N	CYS	G	378	21.621	-10.643	91.610	1.00	18.56	N
ATOM	1492	CA	CYS	G	378	21.156	-10.859	92.961	1.00	19.65	C
ATOM	1493	C	CYS	G	378	19.777	-10.235	93.173	1.00	18.46	C
ATOM	1494	O	CYS	G	378	19.574	-9.041	92.945	1.00	18.50	O
ATOM	1495	CB	CYS	G	378	22.165	-10.299	93.954	1.00	23.94	C
ATOM	1496	SG	CYS	G	378	21.505	-10.141	95.635	1.00	29.07	S
ATOM	1497	N	GLY	G	379	18.822	-11.062	93.580	1.00	17.14	N
ATOM	1498	CA	GLY	G	379	17.473	-10.589	93.825	1.00	14.59	C
ATOM	1499	C	GLY	G	379	16.886	-9.817	92.665	1.00	13.25	C
ATOM	1500	O	GLY	G	379	16.120	-8.879	92.880	1.00	12.24	O
ATOM	1501	N	GLY	G	380	17.228	-10.205	91.439	1.00	13.61	N
ATOM	1502	CA	GLY	G	380	16.716	-9.510	90.265	1.00	14.33	C
ATOM	1503	C	GLY	G	380	17.650	-8.421	89.749	1.00	15.07	C
ATOM	1504	O	GLY	G	380	17.717	-8.171	88.546	1.00	16.13	O
ATOM	1505	N	GLU	G	381	18.383	-7.790	90.663	1.00	14.90	N
ATOM	1506	CA	GLU	G	381	19.332	-6.720	90.353	1.00	13.02	C
ATOM	1507	C	GLU	G	381	20.696	-7.221	89.861	1.00	10.60	C
ATOM	1508	O	GLU	G	381	21.112	-8.338	90.167	1.00	11.59	O
ATOM	1509	CB	GLU	G	381	19.531	-5.847	91.594	1.00	13.97	C
ATOM	1510	CG	GLU	G	381	18.237	-5.322	92.190	1.00	15.75	C
ATOM	1511	CD	GLU	G	381	17.441	-4.452	91.236	1.00	16.89	C
ATOM	1512	OE1	GLU	G	381	18.034	-3.590	90.556	1.00	16.68	O
ATOM	1513	OE2	GLU	G	381	16.202	-4.613	91.183	1.00	16.68	O
ATOM	1514	N	PHE	G	382	21.415	-6.374	89.133	1.00	8.55	N
ATOM	1515	CA	PHE	G	382	22.722	-6.749	88.602	1.00	6.61	C
ATOM	1516	C	PHE	G	382	23.859	-6.180	89.437	1.00	6.22	C
ATOM	1517	O	PHE	G	382	24.055	-4.970	89.471	1.00	6.06	O
ATOM	1518	CB	PHE	G	382	22.860	-6.298	87.142	1.00	5.59	C
ATOM	1519	CG	PHE	G	382	22.107	-7.160	86.169	1.00	3.05	C
ATOM	1520	CD1	PHE	G	382	20.777	-6.906	85.883	1.00	2.75	C
ATOM	1521	CD2	PHE	G	382	22.723	-8.253	85.567	1.00	5.74	C
ATOM	1522	CE1	PHE	G	382	20.065	-7.734	85.011	1.00	7.02	C
ATOM	1523	CE2	PHE	G	382	22.017	-9.093	84.688	1.00	5.25	C
ATOM	1524	CZ	PHE	G	382	20.690	-8.836	84.411	1.00	3.76	C

FIG. 53-30

ATOM	1526	CA	PHE	G	383	25.717	-6.661	90.954	1.00	6.22	C
ATOM	1527	C	PHE	G	383	27.057	-6.759	90.221	1.00	6.64	C
ATOM	1528	O	PHE	G	383	27.267	-7.662	89.415	1.00	7.52	O
ATOM	1529	CB	PHE	G	383	25.791	-7.544	92.199	1.00	6.69	C
ATOM	1530	CG	PHE	G	383	24.766	-7.220	93.251	1.00	7.52	C
ATOM	1531	CD1	PHE	G	383	23.405	-7.274	92.966	1.00	7.11	C
ATOM	1532	CD2	PHE	G	383	25.162	-6.886	94.541	1.00	9.04	C
ATOM	1533	CE1	PHE	G	383	22.449	-7.003	93.950	1.00	5.43	C
ATOM	1534	CE2	PHE	G	383	24.211	-6.612	95.529	1.00	9.60	C
ATOM	1535	CZ	PHE	G	383	22.849	-6.673	95.224	1.00	8.15	C
ATOM	1536	N	TYR	G	384	27.951	-5.814	90.498	1.00	7.28	N
ATOM	1537	CA	TYR	G	384	29.288	-5.792	89.921	1.00	7.20	C
ATOM	1538	C	TYR	G	384	30.192	-5.624	91.123	1.00	9.74	C
ATOM	1539	O	TYR	G	384	30.443	-4.498	91.583	1.00	7.60	O
ATOM	1540	CB	TYR	G	384	29.467	-4.631	88.944	1.00	5.41	C
ATOM	1541	CG	TYR	G	384	28.790	-4.859	87.618	1.00	6.23	C
ATOM	1542	CD1	TYR	G	384	27.397	-4.865	87.519	1.00	7.75	C
ATOM	1543	CD2	TYR	G	384	29.532	-5.138	86.479	1.00	3.64	C
ATOM	1544	CE1	TYR	G	384	26.767	-5.151	86.324	1.00	6.63	C
ATOM	1545	CE2	TYR	G	384	28.910	-5.422	85.285	1.00	5.35	C
ATOM	1546	CZ	TYR	G	384	27.528	-5.435	85.213	1.00	7.83	C
ATOM	1547	OH	TYR	G	384	26.902	-5.754	84.035	1.00	9.77	O
ATOM	1548	N	CYS	G	385	30.596	-6.769	91.672	1.00	11.76	N
ATOM	1549	CA	CYS	G	385	31.444	-6.837	92.855	1.00	13.95	C
ATOM	1550	C	CYS	G	385	32.920	-6.827	92.532	1.00	13.31	C
ATOM	1551	O	CYS	G	385	33.412	-7.713	91.838	1.00	13.77	O
ATOM	1552	CB	CYS	G	385	31.109	-8.095	93.665	1.00	16.62	C
ATOM	1553	SG	CYS	G	385	30.158	-7.819	95.196	1.00	24.71	S
ATOM	1554	N	ASN	G	386	33.617	-5.824	93.054	1.00	14.35	N
ATOM	1555	CA	ASN	G	386	35.061	-5.649	92.875	1.00	14.44	C
ATOM	1556	C	ASN	G	386	35.779	-6.732	93.694	1.00	14.52	C
ATOM	1557	O	ASN	G	386	35.705	-6.730	94.926	1.00	14.97	O
ATOM	1558	CB	ASN	G	386	35.425	-4.231	93.337	1.00	14.08	C
ATOM	1559	CG	ASN	G	386	36.921	-3.995	93.467	1.00	13.06	C
ATOM	1560	OD1	ASN	G	386	37.757	-4.816	93.076	1.00	12.59	O
ATOM	1561	ND2	ASN	G	386	37.244	-2.849	94.062	1.00	13.67	N
ATOM	1562	N	SER	G	387	36.480	-7.637	93.013	1.00	13.53	N
ATOM	1563	CA	SER	G	387	37.143	-8.748	93.689	1.00	12.23	C
ATOM	1564	C	SER	G	387	38.659	-8.732	93.818	1.00	13.58	C
ATOM	1565	O	SER	G	387	39.256	-9.774	94.085	1.00	14.47	O
ATOM	1566	CB	SER	G	387	36.721	-10.068	93.042	1.00	10.53	C
ATOM	1567	OG	SER	G	387	37.183	-10.157	91.706	1.00	5.98	O
ATOM	1568	N	THR	G	388	39.299	-7.575	93.684	1.00	14.06	N
ATOM	1569	CA	THR	G	388	40.758	-7.530	93.794	1.00	13.25	C
ATOM	1570	C	THR	G	388	41.255	-8.269	95.036	1.00	13.29	C
ATOM	1571	O	THR	G	388	42.319	-8.878	95.013	1.00	12.96	O
ATOM	1572	CB	THR	G	388	41.271	-6.078	93.850	1.00	12.91	C
ATOM	1573	OG1	THR	G	388	40.886	-5.391	92.651	1.00	15.59	O
ATOM	1574	CG2	THR	G	388	42.798	-6.044	93.982	1.00	10.34	C
ATOM	1575	N	GLN	G	389	40.456	-8.242	96.101	1.00	14.26	N
ATOM	1576	CA	GLN	G	389	40.806	-8.876	97.377	1.00	15.10	C
ATOM	1577	C	GLN	G	389	40.728	-10.388	97.433	1.00	15.75	C
ATOM	1578	O	GLN	G	389	41.126	-10.991	98.429	1.00	16.29	O
ATOM	1579	CB	GLN	G	389	39.942	-8.331	98.498	1.00	14.13	C
ATOM	1580	CG	GLN	G	389	40.175	-6.895	98.826	1.00	11.93	C
ATOM	1581	CD	GLN	G	389	39.164	-6.419	99.816	1.00	13.44	C
ATOM	1582	OE1	GLN	G	389	38.019	-6.150	99.456	1.00	13.89	O
ATOM	1583	NE2	GLN	G	389	39.547	-6.378	101.087	1.00	12.50	N
ATOM	1584	N	LEU	G	390	40.135	-10.997	96.418	1.00	15.10	N
ATOM	1585	CA	LEU	G	390	40.032	-12.436	96.396	1.00	14.73	C
ATOM	1586	C	LEU	G	390	41.191	-12.988	95.581	1.00	15.84	C
ATOM	1587	O	LEU	G	390	41.787	-14.007	95.941	1.00	15.56	O
ATOM	1588	CB	LEU	G	390	38.686	-12.866	95.812	1.00	15.03	C
ATOM	1589	CG	LEU	G	390	37.446	-12.472	96.628	1.00	14.64	C
ATOM	1590	CD1	LEU	G	390	36.183	-12.891	95.913	1.00	13.49	C
ATOM	1591	CD2	LEU	G	390	37.502	-13.114	97.994	1.00	14.61	C
ATOM	1592	N	PHE	G	391	41.604	-12.235	94.572	1.00	16.01	N
ATOM	1593	CA	PHE	G	391	42.681	-12.675	93.700	1.00	17.41	C
ATOM	1594	C	PHE	G	391	43.886	-11.730	93.729	1.00	21.15	C
ATOM	1595	O	PHE	G	391	44.128	-10.966	92.795	1.00	20.98	O

FIG. 53-31

ATOM	1597	CG	PHE	G	391	40.811	-13.590	92.251	1.00	12.10	C
ATOM	1598	CD1	PHE	G	391	40.781	-14.983	92.260	1.00	11.26	C
ATOM	1599	CD2	PHE	G	391	39.602	-12.895	92.225	1.00	8.89	C
ATOM	1600	CE1	PHE	G	391	39.560	-15.671	92.248	1.00	11.86	C
ATOM	1601	CE2	PHE	G	391	38.383	-13.565	92.215	1.00	6.77	C
ATOM	1602	CZ	PHE	G	391	38.359	-14.955	92.223	1.00	9.67	C
ATOM	1603	N	ASN	G	392	44.632	-11.783	94.826	1.00	24.97	N
ATOM	1604	CA	ASN	G	392	45.813	-10.949	95.012	1.00	28.18	C
ATOM	1605	C	ASN	G	392	46.600	-11.565	96.169	1.00	28.19	C
ATOM	1606	O	ASN	G	392	46.477	-11.153	97.325	1.00	29.12	O
ATOM	1607	CB	ASN	G	392	45.395	-9.506	95.323	1.00	32.77	C
ATOM	1608	CG	ASN	G	392	46.577	-8.546	95.383	1.00	38.54	C
ATOM	1609	OD1	ASN	G	392	47.067	-8.096	94.343	1.00	38.50	O
ATOM	1610	ND2	ASN	G	392	47.055	-8.234	96.588	1.00	43.33	N
ATOM	1611	N	SER	G	393	47.396	-12.577	95.851	1.00	26.88	N
ATOM	1612	CA	SER	G	393	48.180	-13.271	96.857	1.00	25.07	C
ATOM	1613	C	SER	G	393	49.251	-14.104	96.188	1.00	24.68	C
ATOM	1614	O	SER	G	393	49.289	-14.200	94.963	1.00	24.20	O
ATOM	1615	CB	SER	G	393	47.267	-14.178	97.668	1.00	24.54	C
ATOM	1616	OG	SER	G	393	46.466	-14.977	96.815	1.00	24.25	O
ATOM	1617	N	THR	G	394	50.128	-14.695	96.991	1.00	24.89	N
ATOM	1618	CA	THR	G	394	51.188	-15.531	96.457	1.00	25.72	C
ATOM	1619	C	THR	G	394	51.357	-16.790	97.299	1.00	26.39	C
ATOM	1620	O	THR	G	394	51.173	-16.770	98.522	1.00	25.65	O
ATOM	1621	CB	THR	G	394	52.512	-14.781	96.365	1.00	24.64	C
ATOM	1622	OG1	THR	G	394	52.287	-13.492	95.782	1.00	24.17	O
ATOM	1623	CG2	THR	G	394	53.471	-15.548	95.485	1.00	24.29	C
ATOM	1624	N	TRP	G	395	51.654	-17.890	96.613	1.00	26.26	N
ATOM	1625	CA	TRP	G	395	51.832	-19.191	97.235	1.00	25.14	C
ATOM	1626	C	TRP	G	395	52.914	-19.942	96.475	1.00	26.41	C
ATOM	1627	O	TRP	G	395	53.501	-19.434	95.510	1.00	26.05	O
ATOM	1628	CB	TRP	G	395	50.543	-20.022	97.138	1.00	22.22	C
ATOM	1629	CG	TRP	G	395	49.262	-19.274	97.377	1.00	19.31	C
ATOM	1630	CD1	TRP	G	395	48.617	-18.447	96.497	1.00	16.61	C
ATOM	1631	CD2	TRP	G	395	48.454	-19.308	98.562	1.00	16.61	C
ATOM	1632	NE1	TRP	G	395	47.463	-17.969	97.062	1.00	16.86	N
ATOM	1633	CE2	TRP	G	395	47.336	-18.479	98.328	1.00	14.88	C
ATOM	1634	CE3	TRP	G	395	48.566	-19.956	99.798	1.00	16.95	C
ATOM	1635	CZ2	TRP	G	395	46.334	-18.286	99.280	1.00	12.10	C
ATOM	1636	CZ3	TRP	G	395	47.560	-19.761	100.752	1.00	15.27	C
ATOM	1637	CH2	TRP	G	395	46.463	-18.931	100.482	1.00	14.32	C
ATOM	1638	N	PHE	G	396	53.155	-21.174	96.902	1.00	27.88	N
ATOM	1639	CA	PHE	G	396	54.145	-22.031	96.262	1.00	28.86	C
ATOM	1640	C	PHE	G	396	53.534	-23.428	96.176	1.00	27.43	C
ATOM	1641	O	PHE	G	396	52.313	-23.576	96.300	1.00	26.00	O
ATOM	1642	CB	PHE	G	396	55.458	-22.043	97.066	1.00	30.01	C
ATOM	1643	CG	PHE	G	396	56.096	-20.681	97.217	1.00	29.71	C
ATOM	1644	CD1	PHE	G	396	56.966	-20.200	96.256	1.00	30.49	C
ATOM	1645	CD2	PHE	G	396	55.815	-19.880	98.316	1.00	31.10	C
ATOM	1646	CE1	PHE	G	396	57.549	-18.939	96.379	1.00	31.47	C
ATOM	1647	CE2	PHE	G	396	56.396	-18.613	98.447	1.00	32.07	C
ATOM	1648	CZ	PHE	G	396	57.262	-18.146	97.475	1.00	30.57	C
ATOM	1649	N	GLY	G	410	39.849	-12.755	114.824	1.00	52.61	N
ATOM	1650	CA	GLY	G	410	38.587	-13.108	115.447	1.00	52.39	C
ATOM	1651	C	GLY	G	410	37.505	-13.439	114.438	1.00	52.68	C
ATOM	1652	O	GLY	G	410	37.211	-14.611	114.187	1.00	52.57	O
ATOM	1653	N	SER	G	411	36.904	-12.405	113.859	1.00	52.15	N
ATOM	1654	CA	SER	G	411	35.853	-12.596	112.868	1.00	50.82	C
ATOM	1655	C	SER	G	411	36.158	-11.719	111.649	1.00	49.37	C
ATOM	1656	O	SER	G	411	35.352	-10.878	111.241	1.00	49.20	O
ATOM	1657	CB	SER	G	411	34.488	-12.252	113.479	1.00	50.78	C
ATOM	1658	OG	SER	G	411	33.416	-12.697	112.661	1.00	52.19	O
ATOM	1659	N	ASP	G	412	37.344	-11.920	111.087	1.00	47.75	N
ATOM	1660	CA	ASP	G	412	37.805	-11.170	109.923	1.00	46.28	C
ATOM	1661	C	ASP	G	412	37.092	-11.612	108.649	1.00	44.08	C
ATOM	1662	O	ASP	G	412	37.242	-12.761	108.214	1.00	44.81	O
ATOM	1663	CB	ASP	G	412	39.312	-11.373	109.738	1.00	49.02	C
ATOM	1664	CG	ASP	G	412	40.144	-10.671	110.801	1.00	51.99	C
ATOM	1665	OD1	ASP	G	412	40.479	-9.476	110.608	1.00	53.47	O
ATOM	1666	OD2	ASP	G	412	40.486	-11.324	111.811	1.00	54.16	O

FIG. 53-32

ATOM	1668	CA	THR	G	413	35.584	-11.026	106.828	1.00	35.17	C
ATOM	1669	C	THR	G	413	36.110	-10.208	105.646	1.00	32.12	C
ATOM	1670	O	THR	G	413	36.544	-9.060	105.808	1.00	31.22	O
ATOM	1671	CB	THR	G	413	34.054	-10.813	106.972	1.00	33.87	C
ATOM	1672	OG1	THR	G	413	33.792	-9.594	107.672	1.00	32.02	O
ATOM	1673	CG2	THR	G	413	33.429	-11.959	107.732	1.00	34.44	C
ATOM	1674	N	ILE	G	414	36.159	-10.843	104.479	1.00	28.34	N
ATOM	1675	CA	ILE	G	414	36.614	-10.187	103.268	1.00	24.52	C
ATOM	1676	C	ILE	G	414	35.458	-9.380	102.705	1.00	22.34	C
ATOM	1677	O	ILE	G	414	34.510	-9.945	102.153	1.00	20.15	O
ATOM	1678	CB	ILE	G	414	37.067	-11.193	102.190	1.00	24.43	C
ATOM	1679	CG1	ILE	G	414	38.277	-11.992	102.671	1.00	23.83	C
ATOM	1680	CG2	ILE	G	414	37.413	-10.455	100.908	1.00	23.71	C
ATOM	1681	CD1	ILE	G	414	38.858	-12.924	101.622	1.00	23.64	C
ATOM	1682	N	THR	G	415	35.510	-8.066	102.921	1.00	21.24	N
ATOM	1683	CA	THR	G	415	34.487	-7.161	102.417	1.00	19.23	C
ATOM	1684	C	THR	G	415	34.843	-6.756	100.989	1.00	18.99	C
ATOM	1685	O	THR	G	415	35.941	-6.267	100.726	1.00	19.68	O
ATOM	1686	CB	THR	G	415	34.359	-5.913	103.301	1.00	17.55	C
ATOM	1687	OG1	THR	G	415	33.746	-6.276	104.542	1.00	18.24	O
ATOM	1688	CG2	THR	G	415	33.519	-4.857	102.627	1.00	16.11	C
ATOM	1689	N	LEU	G	416	33.923	-7.010	100.070	1.00	16.60	N
ATOM	1690	CA	LEU	G	416	34.114	-6.680	98.665	1.00	14.46	C
ATOM	1691	C	LEU	G	416	33.161	-5.564	98.278	1.00	12.35	C
ATOM	1692	O	LEU	G	416	31.959	-5.635	98.573	1.00	9.32	O
ATOM	1693	CB	LEU	G	416	33.799	-7.902	97.797	1.00	15.19	C
ATOM	1694	CG	LEU	G	416	34.873	-8.761	97.133	1.00	14.82	C
ATOM	1695	CD1	LEU	G	416	36.074	-8.962	98.035	1.00	17.46	C
ATOM	1696	CD2	LEU	G	416	34.250	-10.088	96.759	1.00	13.29	C
ATOM	1697	N	PRO	G	417	33.694	-4.480	97.686	1.00	11.52	N
ATOM	1698	CA	PRO	G	417	32.875	-3.348	97.251	1.00	11.96	C
ATOM	1699	C	PRO	G	417	32.049	-3.903	96.094	1.00	12.68	C
ATOM	1700	O	PRO	G	417	32.588	-4.602	95.228	1.00	12.98	O
ATOM	1701	CB	PRO	G	417	33.914	-2.352	96.724	1.00	12.10	C
ATOM	1702	CG	PRO	G	417	35.173	-2.740	97.406	1.00	11.06	C
ATOM	1703	CD	PRO	G	417	35.117	-4.228	97.412	1.00	11.57	C
ATOM	1704	N	CYS	G	418	30.785	-3.525	96.025	1.00	13.47	N
ATOM	1705	CA	CYS	G	418	29.897	-4.023	94.992	1.00	15.31	C
ATOM	1706	C	CYS	G	418	29.086	-2.853	94.435	1.00	16.22	C
ATOM	1707	O	CYS	G	418	28.928	-1.832	95.101	1.00	17.53	O
ATOM	1708	CB	CYS	G	418	28.964	-5.049	95.618	1.00	16.68	C
ATOM	1709	SG	CYS	G	418	28.665	-6.556	94.655	1.00	21.94	S
ATOM	1710	N	ARG	G	419	28.585	-2.992	93.211	1.00	16.78	N
ATOM	1711	CA	ARG	G	419	27.794	-1.932	92.582	1.00	16.62	C
ATOM	1712	C	ARG	G	419	26.685	-2.521	91.720	1.00	16.08	C
ATOM	1713	O	ARG	G	419	26.903	-3.504	91.021	1.00	16.64	O
ATOM	1714	CB	ARG	G	419	28.678	-1.007	91.717	1.00	15.68	C
ATOM	1715	CG	ARG	G	419	27.936	0.239	91.257	1.00	20.03	C
ATOM	1716	CD	ARG	G	419	28.752	1.214	90.415	1.00	24.39	C
ATOM	1717	NE	ARG	G	419	27.968	2.426	90.131	1.00	29.10	N
ATOM	1718	CZ	ARG	G	419	28.476	3.651	89.974	1.00	30.37	C
ATOM	1719	NH1	ARG	G	419	29.785	3.855	90.060	1.00	29.71	N
ATOM	1720	NH2	ARG	G	419	27.664	4.697	89.829	1.00	29.99	N
ATOM	1721	N	ILE	G	420	25.502	-1.919	91.782	1.00	15.40	N
ATOM	1722	CA	ILE	G	420	24.355	-2.359	91.001	1.00	13.99	C
ATOM	1723	C	ILE	G	420	24.247	-1.458	89.773	1.00	15.21	C
ATOM	1724	O	ILE	G	420	23.988	-0.256	89.900	1.00	17.67	O
ATOM	1725	CB	ILE	G	420	23.070	-2.217	91.808	1.00	13.88	C
ATOM	1726	CG1	ILE	G	420	23.269	-2.795	93.211	1.00	15.98	C
ATOM	1727	CG2	ILE	G	420	21.924	-2.926	91.115	1.00	11.82	C
ATOM	1728	CD1	ILE	G	420	22.137	-2.455	94.195	1.00	19.11	C
ATOM	1729	N	LYS	G	421	24.487	-2.021	88.593	1.00	13.87	N
ATOM	1730	CA	LYS	G	421	24.405	-1.255	87.356	1.00	11.70	C
ATOM	1731	C	LYS	G	421	23.091	-1.534	86.641	1.00	13.43	C
ATOM	1732	O	LYS	G	421	22.480	-2.591	86.828	1.00	14.32	O
ATOM	1733	CB	LYS	G	421	25.583	-1.585	86.443	1.00	8.86	C
ATOM	1734	CG	LYS	G	421	26.930	-1.279	87.064	1.00	5.47	C
ATOM	1735	CD	LYS	G	421	28.061	-1.414	86.066	1.00	2.59	C
ATOM	1736	CE	LYS	G	421	29.387	-1.115	86.741	1.00	2.00	C
ATOM	1737	NZ	LYS	G	421	30.474	-0.802	85.774	1.00	2.10	N

FIG. 53-33

ATOM	1739	CA	GLN	G	422	21.397	-0.709	85.101	1.00	13.90	C
ATOM	1740	C	GLN	G	422	21.673	-0.955	83.610	1.00	14.50	C
ATOM	1741	O	GLN	G	422	20.943	-1.713	82.958	1.00	15.64	O
ATOM	1742	CB	GLN	G	422	20.494	0.506	85.322	1.00	12.83	C
ATOM	1743	CG	GLN	G	422	19.847	0.535	86.717	1.00	14.26	C
ATOM	1744	CD	GLN	G	422	20.518	1.500	87.700	1.00	14.75	C
ATOM	1745	OE1	GLN	G	422	20.787	2.652	87.368	1.00	16.42	O
ATOM	1746	NE2	GLN	G	422	20.765	1.035	88.921	1.00	13.83	N
ATOM	1747	N	ILE	G	423	22.732	-0.339	83.085	1.00	13.65	N
ATOM	1748	CA	ILE	G	423	23.129	-0.515	81.686	1.00	12.75	C
ATOM	1749	C	ILE	G	423	24.195	-1.611	81.697	1.00	12.32	C
ATOM	1750	O	ILE	G	423	25.281	-1.415	82.239	1.00	12.02	O
ATOM	1751	CB	ILE	G	423	23.814	0.744	81.086	1.00	12.86	C
ATOM	1752	CG1	ILE	G	423	23.001	2.025	81.344	1.00	13.94	C
ATOM	1753	CG2	ILE	G	423	24.057	0.529	79.614	1.00	12.18	C
ATOM	1754	CD1	ILE	G	423	21.708	2.151	80.554	1.00	14.57	C
ATOM	1755	N	ILE	G	424	23.912	-2.743	81.063	1.00	11.96	N
ATOM	1756	CA	ILE	G	424	24.867	-3.850	81.036	1.00	10.17	C
ATOM	1757	C	ILE	G	424	25.153	-4.381	79.639	1.00	9.57	C
ATOM	1758	O	ILE	G	424	24.355	-4.202	78.719	1.00	10.04	O
ATOM	1759	CB	ILE	G	424	24.346	-5.031	81.881	1.00	6.45	C
ATOM	1760	CG1	ILE	G	424	22.906	-5.363	81.463	1.00	6.31	C
ATOM	1761	CG2	ILE	G	424	24.379	-4.671	83.343	1.00	4.81	C
ATOM	1762	CD1	ILE	G	424	22.384	-6.680	81.976	1.00	5.79	C
ATOM	1763	N	ASN	G	425	26.325	-4.980	79.471	1.00	10.25	N
ATOM	1764	CA	ASN	G	425	26.692	-5.611	78.204	1.00	10.60	C
ATOM	1765	C	ASN	G	425	26.048	-6.998	78.349	1.00	10.47	C
ATOM	1766	O	ASN	G	425	26.174	-7.641	79.400	1.00	10.16	O
ATOM	1767	CB	ASN	G	425	28.212	-5.763	78.090	1.00	12.33	C
ATOM	1768	CG	ASN	G	425	28.939	-4.427	78.007	1.00	15.15	C
ATOM	1769	OD1	ASN	G	425	28.652	-3.607	77.130	1.00	17.02	O
ATOM	1770	ND2	ASN	G	425	29.903	-4.213	78.898	1.00	12.02	N
ATOM	1771	N	MET	G	426	25.319	-7.444	77.335	1.00	11.26	N
ATOM	1772	CA	MET	G	426	24.661	-8.752	77.411	1.00	11.94	C
ATOM	1773	C	MET	G	426	25.623	-9.929	77.323	1.00	11.81	C
ATOM	1774	O	MET	G	426	26.686	-9.839	76.694	1.00	10.19	O
ATOM	1775	CB	MET	G	426	23.612	-8.910	76.305	1.00	11.27	C
ATOM	1776	CG	MET	G	426	22.518	-7.882	76.300	1.00	11.33	C
ATOM	1777	SD	MET	G	426	21.617	-7.901	74.730	1.00	12.85	S
ATOM	1778	CE	MET	G	426	20.042	-8.430	75.332	1.00	13.82	C
ATOM	1779	N	TRP	G	427	25.226	-11.030	77.961	1.00	12.45	N
ATOM	1780	CA	TRP	G	427	25.995	-12.273	77.938	1.00	11.41	C
ATOM	1781	C	TRP	G	427	25.385	-13.206	76.878	1.00	11.82	C
ATOM	1782	O	TRP	G	427	26.056	-14.083	76.348	1.00	11.82	O
ATOM	1783	CB	TRP	G	427	25.977	-12.954	79.319	1.00	10.11	C
ATOM	1784	CG	TRP	G	427	24.631	-13.502	79.756	1.00	7.53	C
ATOM	1785	CD1	TRP	G	427	23.711	-12.877	80.542	1.00	8.23	C
ATOM	1786	CD2	TRP	G	427	24.046	-14.769	79.392	1.00	7.92	C
ATOM	1787	NE1	TRP	G	427	22.589	-13.658	80.684	1.00	8.61	N
ATOM	1788	CE2	TRP	G	427	22.765	-14.824	79.988	1.00	7.83	C
ATOM	1789	CE3	TRP	G	427	24.477	-15.860	78.617	1.00	4.40	C
ATOM	1790	CZ2	TRP	G	427	21.907	-15.927	79.834	1.00	4.16	C
ATOM	1791	CZ3	TRP	G	427	23.626	-16.953	78.466	1.00	3.07	C
ATOM	1792	CH2	TRP	G	427	22.354	-16.974	79.074	1.00	3.36	C
ATOM	1793	N	GLN	G	428	24.102	-13.002	76.578	1.00	12.92	N
ATOM	1794	CA	GLN	G	428	23.383	-13.819	75.602	1.00	12.50	C
ATOM	1795	C	GLN	G	428	23.995	-13.688	74.226	1.00	12.17	C
ATOM	1796	O	GLN	G	428	24.340	-14.686	73.592	1.00	12.46	O
ATOM	1797	CB	GLN	G	428	21.907	-13.410	75.532	1.00	13.40	C
ATOM	1798	CG	GLN	G	428	21.076	-13.744	76.776	1.00	17.89	C
ATOM	1799	CD	GLN	G	428	20.660	-12.520	77.570	1.00	17.31	C
ATOM	1800	OE1	GLN	G	428	21.457	-11.608	77.793	1.00	19.51	O
ATOM	1801	NE2	GLN	G	428	19.418	-12.501	78.012	1.00	16.89	N
ATOM	1802	N	LYS	G	429	24.126	-12.440	73.781	1.00	12.47	N
ATOM	1803	CA	LYS	G	429	24.676	-12.096	72.472	1.00	11.30	C
ATOM	1804	C	LYS	G	429	25.355	-10.737	72.649	1.00	11.73	C
ATOM	1805	O	LYS	G	429	25.245	-10.134	73.720	1.00	11.55	O
ATOM	1806	CB	LYS	G	429	23.541	-12.013	71.443	1.00	10.96	C
ATOM	1807	CG	LYS	G	429	22.583	-10.847	71.655	1.00	10.29	C
ATOM	1808	CD	LYS	G	429	21.234	-11.049	70.963	1.00	9.65	C

FIG. 53-34

ATOM	1810	NZ	LYS	G	429	18.772	-11.467	71.526	1.00	14.65	N
ATOM	1811	N	VAL	G	430	26.075	-10.266	71.630	1.00	12.29	N
ATOM	1812	CA	VAL	G	430	26.763	-8.976	71.727	1.00	11.03	C
ATOM	1813	C	VAL	G	430	25.778	-7.819	71.695	1.00	12.15	C
ATOM	1814	O	VAL	G	430	25.471	-7.269	70.635	1.00	13.94	O
ATOM	1815	CB	VAL	G	430	27.835	-8.792	70.629	1.00	9.34	C
ATOM	1816	CG1	VAL	G	430	28.306	-7.345	70.578	1.00	7.26	C
ATOM	1817	CG2	VAL	G	430	29.025	-9.687	70.908	1.00	7.39	C
ATOM	1818	N	GLY	G	431	25.288	-7.450	72.869	1.00	11.73	N
ATOM	1819	CA	GLY	G	431	24.335	-6.364	72.956	1.00	11.01	C
ATOM	1820	C	GLY	G	431	24.505	-5.575	74.235	1.00	10.82	C
ATOM	1821	O	GLY	G	431	25.433	-5.820	75.027	1.00	9.94	O
ATOM	1822	N	LYS	G	432	23.594	-4.630	74.432	1.00	9.68	N
ATOM	1823	CA	LYS	G	432	23.583	-3.761	75.597	1.00	10.19	C
ATOM	1824	C	LYS	G	432	22.130	-3.740	76.066	1.00	10.15	C
ATOM	1825	O	LYS	G	432	21.218	-3.913	75.251	1.00	11.95	O
ATOM	1826	CB	LYS	G	432	24.021	-2.355	75.168	1.00	12.15	C
ATOM	1827	CG	LYS	G	432	24.193	-1.330	76.284	1.00	12.45	C
ATOM	1828	CD	LYS	G	432	25.407	-1.624	77.142	1.00	13.71	C
ATOM	1829	CE	LYS	G	432	26.671	-1.729	76.308	1.00	14.39	C
ATOM	1830	NZ	LYS	G	432	26.857	-0.585	75.395	1.00	16.43	N
ATOM	1831	N	ALA	G	433	21.904	-3.576	77.364	1.00	8.77	N
ATOM	1832	CA	ALA	G	433	20.544	-3.536	77.889	1.00	7.95	C
ATOM	1833	C	ALA	G	433	20.465	-2.606	79.095	1.00	8.53	C
ATOM	1834	O	ALA	G	433	21.481	-2.329	79.734	1.00	9.95	O
ATOM	1835	CB	ALA	G	433	20.076	-4.933	78.253	1.00	5.09	C
ATOM	1836	N	MET	G	434	19.273	-2.082	79.367	1.00	8.52	N
ATOM	1837	CA	MET	G	434	19.063	-1.176	80.492	1.00	8.68	C
ATOM	1838	C	MET	G	434	17.835	-1.608	81.263	1.00	8.39	C
ATOM	1839	O	MET	G	434	16.775	-1.822	80.674	1.00	10.62	O
ATOM	1840	CB	MET	G	434	18.860	0.260	79.993	1.00	12.16	C
ATOM	1841	CG	MET	G	434	18.402	1.263	81.072	1.00	13.05	C
ATOM	1842	SD	MET	G	434	18.040	2.931	80.444	1.00	14.02	S
ATOM	1843	CE	MET	G	434	16.368	2.691	79.882	1.00	7.69	C
ATOM	1844	N	TYR	G	435	17.980	-1.758	82.570	1.00	6.27	N
ATOM	1845	CA	TYR	G	435	16.868	-2.156	83.409	1.00	7.78	C
ATOM	1846	C	TYR	G	435	16.482	-1.020	84.369	1.00	9.51	C
ATOM	1847	O	TYR	G	435	17.229	-0.060	84.556	1.00	8.60	O
ATOM	1848	CB	TYR	G	435	17.221	-3.423	84.192	1.00	8.02	C
ATOM	1849	CG	TYR	G	435	17.475	-4.648	83.334	1.00	6.79	C
ATOM	1850	CD1	TYR	G	435	18.682	-4.811	82.646	1.00	7.18	C
ATOM	1851	CD2	TYR	G	435	16.513	-5.648	83.218	1.00	6.66	C
ATOM	1852	CE1	TYR	G	435	18.922	-5.939	81.862	1.00	3.85	C
ATOM	1853	CE2	TYR	G	435	16.745	-6.785	82.435	1.00	6.36	C
ATOM	1854	CZ	TYR	G	435	17.950	-6.919	81.761	1.00	4.00	C
ATOM	1855	OH	TYR	G	435	18.160	-8.019	80.975	1.00	2.00	O
ATOM	1856	N	ALA	G	436	15.299	-1.119	84.958	1.00	10.38	N
ATOM	1857	CA	ALA	G	436	14.840	-0.104	85.891	1.00	11.10	C
ATOM	1858	C	ALA	G	436	15.688	-0.137	87.162	1.00	11.27	C
ATOM	1859	O	ALA	G	436	16.372	-1.126	87.435	1.00	11.03	O
ATOM	1860	CB	ALA	G	436	13.388	-0.347	86.234	1.00	9.64	C
ATOM	1861	N	PRO	G	437	15.711	0.972	87.914	1.00	11.91	N
ATOM	1862	CA	PRO	G	437	16.489	1.027	89.160	1.00	11.96	C
ATOM	1863	C	PRO	G	437	15.778	0.190	90.231	1.00	14.06	C
ATOM	1864	O	PRO	G	437	14.629	-0.223	90.041	1.00	14.86	O
ATOM	1865	CB	PRO	G	437	16.466	2.519	89.509	1.00	10.51	C
ATOM	1866	CG	PRO	G	437	16.373	3.175	88.165	1.00	11.89	C
ATOM	1867	CD	PRO	G	437	15.327	2.328	87.482	1.00	11.18	C
ATOM	1868	N	PRO	G	438	16.447	-0.084	91.364	1.00	15.61	N
ATOM	1869	CA	PRO	G	438	15.808	-0.878	92.409	1.00	16.39	C
ATOM	1870	C	PRO	G	438	14.573	-0.220	93.012	1.00	17.69	C
ATOM	1871	O	PRO	G	438	14.380	0.990	92.898	1.00	19.30	O
ATOM	1872	CB	PRO	G	438	16.908	-0.988	93.466	1.00	15.98	C
ATOM	1873	CG	PRO	G	438	18.166	-0.894	92.676	1.00	15.96	C
ATOM	1874	CD	PRO	G	438	17.846	0.215	91.724	1.00	15.89	C
ATOM	1875	N	ILE	G	439	13.729	-1.042	93.628	1.00	17.73	N
ATOM	1876	CA	ILE	G	439	12.528	-0.583	94.320	1.00	18.43	C
ATOM	1877	C	ILE	G	439	12.611	-1.061	95.772	1.00	20.45	C
ATOM	1878	O	ILE	G	439	12.038	-0.457	96.675	1.00	21.24	O
ATOM	1879	CB	ILE	G	439	11.246	-1.135	93.697	1.00	17.29	C

FIG. 53-35

ATOM	1881	CG2	ILE	G	439	10.967	-0.438	92.389	1.00	18.43	C
ATOM	1882	CD1	ILE	G	439	10.104	-3.259	92.950	1.00	18.43	C
ATOM	1883	N	SER	G	440	13.349	-2.148	95.984	1.00	21.82	N
ATOM	1884	CA	SER	G	440	13.536	-2.723	97.306	1.00	21.89	C
ATOM	1885	C	SER	G	440	14.721	-2.063	97.992	1.00	22.21	C
ATOM	1886	O	SER	G	440	15.688	-1.671	97.334	1.00	21.84	O
ATOM	1887	CB	SER	G	440	13.787	-4.224	97.182	1.00	22.41	C
ATOM	1888	OG	SER	G	440	14.322	-4.774	98.376	1.00	24.55	O
ATOM	1889	N	GLY	G	441	14.645	-1.963	99.316	1.00	22.89	N
ATOM	1890	CA	GLY	G	441	15.717	-1.364	100.087	1.00	24.15	C
ATOM	1891	C	GLY	G	441	16.437	-2.406	100.918	1.00	25.78	C
ATOM	1892	O	GLY	G	441	17.183	-2.083	101.850	1.00	25.75	O
ATOM	1893	N	GLN	G	442	16.223	-3.669	100.565	1.00	27.91	N
ATOM	1894	CA	GLN	G	442	16.835	-4.791	101.271	1.00	27.60	C
ATOM	1895	C	GLN	G	442	17.094	-5.945	100.305	1.00	26.17	C
ATOM	1896	O	GLN	G	442	16.502	-7.011	100.433	1.00	25.20	O
ATOM	1897	CB	GLN	G	442	15.919	-5.256	102.413	1.00	27.55	C
ATOM	1898	CG	GLN	G	442	16.520	-5.156	103.818	1.00	30.75	C
ATOM	1899	CD	GLN	G	442	17.699	-6.102	104.055	1.00	32.94	C
ATOM	1900	OE1	GLN	G	442	18.557	-5.851	104.913	1.00	33.70	O
ATOM	1901	NE2	GLN	G	442	17.744	-7.191	103.302	1.00	32.33	N
ATOM	1902	N	ILE	G	443	17.917	-5.691	99.291	1.00	25.88	N
ATOM	1903	CA	ILE	G	443	18.284	-6.717	98.309	1.00	25.15	C
ATOM	1904	C	ILE	G	443	19.295	-7.570	99.094	1.00	25.50	C
ATOM	1905	O	ILE	G	443	20.334	-7.059	99.526	1.00	25.38	O
ATOM	1906	CB	ILE	G	443	18.978	-6.092	97.062	1.00	24.00	C
ATOM	1907	CG1	ILE	G	443	18.131	-4.955	96.465	1.00	22.92	C
ATOM	1908	CG2	ILE	G	443	19.268	-7.158	96.029	1.00	24.67	C
ATOM	1909	CD1	ILE	G	443	16.814	-5.382	95.843	1.00	18.91	C
ATOM	1910	N	ARG	G	444	18.988	-8.845	99.295	1.00	25.73	N
ATOM	1911	CA	ARG	G	444	19.844	-9.719	100.090	1.00	24.77	C
ATOM	1912	C	ARG	G	444	20.013	-11.113	99.508	1.00	23.92	C
ATOM	1913	O	ARG	G	444	19.042	-11.862	99.390	1.00	23.58	O
ATOM	1914	CB	ARG	G	444	19.250	-9.830	101.498	1.00	26.54	C
ATOM	1915	CG	ARG	G	444	17.726	-9.982	101.485	1.00	30.41	C
ATOM	1916	CD	ARG	G	444	17.125	-10.040	102.877	1.00	33.05	C
ATOM	1917	NE	ARG	G	444	17.435	-11.298	103.545	1.00	37.05	N
ATOM	1918	CZ	ARG	G	444	17.082	-11.597	104.789	1.00	37.64	C
ATOM	1919	NH1	ARG	G	444	16.403	-10.723	105.522	1.00	39.42	N
ATOM	1920	NH2	ARG	G	444	17.411	-12.776	105.291	1.00	37.67	N
ATOM	1921	N	CYS	G	445	21.251	-11.474	99.185	1.00	23.87	N
ATOM	1922	CA	CYS	G	445	21.550	-12.791	98.634	1.00	23.58	C
ATOM	1923	C	CYS	G	445	22.575	-13.530	99.472	1.00	22.82	C
ATOM	1924	O	CYS	G	445	23.410	-12.918	100.147	1.00	23.70	O
ATOM	1925	CB	CYS	G	445	22.060	-12.682	97.195	1.00	25.38	C
ATOM	1926	SG	CYS	G	445	20.832	-12.019	96.022	1.00	31.32	S
ATOM	1927	N	SER	G	446	22.485	-14.853	99.456	1.00	21.52	N
ATOM	1928	CA	SER	G	446	23.421	-15.696	100.185	1.00	19.95	C
ATOM	1929	C	SER	G	446	23.700	-16.850	99.253	1.00	17.57	C
ATOM	1930	O	SER	G	446	22.868	-17.742	99.097	1.00	18.36	O
ATOM	1931	CB	SER	G	446	22.794	-16.200	101.485	1.00	22.42	C
ATOM	1932	OG	SER	G	446	22.326	-15.120	102.285	1.00	28.19	O
ATOM	1933	N	SER	G	447	24.832	-16.787	98.566	1.00	15.58	N
ATOM	1934	CA	SER	G	447	25.202	-17.837	97.632	1.00	13.44	C
ATOM	1935	C	SER	G	447	26.382	-18.658	98.123	1.00	12.68	C
ATOM	1936	O	SER	G	447	27.125	-18.248	99.004	1.00	10.83	O
ATOM	1937	CB	SER	G	447	25.499	-17.260	96.241	1.00	11.95	C
ATOM	1938	OG	SER	G	447	24.318	-17.164	95.462	1.00	5.00	O
ATOM	1939	N	ASN	G	448	26.502	-19.857	97.583	1.00	14.33	N
ATOM	1940	CA	ASN	G	448	27.592	-20.732	97.944	1.00	16.20	C
ATOM	1941	C	ASN	G	448	28.564	-20.854	96.769	1.00	14.81	C
ATOM	1942	O	ASN	G	448	28.198	-21.316	95.682	1.00	12.34	O
ATOM	1943	CB	ASN	G	448	27.063	-22.108	98.375	1.00	20.92	C
ATOM	1944	CG	ASN	G	448	26.868	-22.214	99.891	1.00	27.83	C
ATOM	1945	OD1	ASN	G	448	27.851	-22.275	100.635	1.00	26.42	O
ATOM	1946	ND2	ASN	G	448	25.612	-22.222	100.347	1.00	33.87	N
ATOM	1947	N	ILE	G	449	29.767	-20.316	96.948	1.00	12.69	N
ATOM	1948	CA	ILE	G	449	30.771	-20.423	95.916	1.00	10.25	C
ATOM	1949	C	ILE	G	449	31.025	-21.918	95.872	1.00	10.75	C
ATOM	1950	O	ILE	G	449	31.228	-22.565	96.897	1.00	9.42	O

FIG. 53-36

ATOM	1952	CG1	ILE	G	449	31.801	-18.194	96.450	1.00	8.41	C
ATOM	1953	CG2	ILE	G	449	33.103	-19.885	95.166	1.00	6.30	C
ATOM	1954	CD1	ILE	G	449	33.069	-17.378	96.702	1.00	8.72	C
ATOM	1955	N	THR	G	450	30.879	-22.460	94.680	1.00	12.00	N
ATOM	1956	CA	THR	G	450	31.054	-23.871	94.419	1.00	11.69	C
ATOM	1957	C	THR	G	450	32.246	-24.034	93.475	1.00	11.98	C
ATOM	1958	O	THR	G	450	32.760	-25.135	93.291	1.00	13.25	O
ATOM	1959	CB	THR	G	450	29.765	-24.414	93.770	1.00	13.06	C
ATOM	1960	OG1	THR	G	450	28.777	-24.683	94.788	1.00	12.93	O
ATOM	1961	CG2	THR	G	450	30.047	-25.633	92.922	1.00	13.57	C
ATOM	1962	N	GLY	G	451	32.712	-22.928	92.906	1.00	11.41	N
ATOM	1963	CA	GLY	G	451	33.839	-23.018	92.004	1.00	10.26	C
ATOM	1964	C	GLY	G	451	34.587	-21.735	91.708	1.00	8.61	C
ATOM	1965	O	GLY	G	451	34.510	-20.749	92.440	1.00	8.05	O
ATOM	1966	N	LEU	G	452	35.291	-21.757	90.587	1.00	7.27	N
ATOM	1967	CA	LEU	G	452	36.095	-20.640	90.148	1.00	7.77	C
ATOM	1968	C	LEU	G	452	36.388	-20.911	88.677	1.00	6.70	C
ATOM	1969	O	LEU	G	452	36.413	-22.062	88.253	1.00	6.47	O
ATOM	1970	CB	LEU	G	452	37.411	-20.612	90.952	1.00	8.63	C
ATOM	1971	CG	LEU	G	452	37.922	-19.306	91.574	1.00	9.19	C
ATOM	1972	CD1	LEU	G	452	39.244	-19.531	92.278	1.00	7.11	C
ATOM	1973	CD2	LEU	G	452	38.097	-18.258	90.504	1.00	9.43	C
ATOM	1974	N	LEU	G	453	36.505	-19.847	87.892	1.00	5.67	N
ATOM	1975	CA	LEU	G	453	36.823	-19.944	86.475	1.00	4.79	C
ATOM	1976	C	LEU	G	453	38.035	-19.035	86.334	1.00	5.84	C
ATOM	1977	O	LEU	G	453	37.913	-17.824	86.487	1.00	5.97	O
ATOM	1978	CB	LEU	G	453	35.688	-19.382	85.635	1.00	4.15	C
ATOM	1979	CG	LEU	G	453	34.367	-20.112	85.431	1.00	3.40	C
ATOM	1980	CD1	LEU	G	453	33.321	-19.110	84.932	1.00	2.00	C
ATOM	1981	CD2	LEU	G	453	34.556	-21.226	84.431	1.00	4.15	C
ATOM	1982	N	LEU	G	454	39.206	-19.606	86.084	1.00	6.21	N
ATOM	1983	CA	LEU	G	454	40.424	-18.815	85.975	1.00	6.68	C
ATOM	1984	C	LEU	G	454	41.013	-18.696	84.571	1.00	9.91	C
ATOM	1985	O	LEU	G	454	40.426	-19.144	83.577	1.00	8.93	O
ATOM	1986	CB	LEU	G	454	41.488	-19.417	86.876	1.00	5.38	C
ATOM	1987	CG	LEU	G	454	41.157	-19.607	88.345	1.00	5.22	C
ATOM	1988	CD1	LEU	G	454	42.155	-20.577	88.956	1.00	3.11	C
ATOM	1989	CD2	LEU	G	454	41.188	-18.260	89.039	1.00	2.50	C
ATOM	1990	N	THR	G	455	42.212	-18.122	84.535	1.00	13.23	N
ATOM	1991	CA	THR	G	455	42.994	-17.909	83.328	1.00	16.95	C
ATOM	1992	C	THR	G	455	44.440	-17.694	83.785	1.00	20.50	C
ATOM	1993	O	THR	G	455	44.679	-17.180	84.883	1.00	23.09	O
ATOM	1994	CB	THR	G	455	42.460	-16.695	82.546	1.00	16.91	C
ATOM	1995	OG1	THR	G	455	41.680	-17.158	81.434	1.00	19.13	O
ATOM	1996	CG2	THR	G	455	43.585	-15.798	82.051	1.00	17.25	C
ATOM	1997	N	ARG	G	456	45.408	-18.091	82.967	1.00	22.71	N
ATOM	1998	CA	ARG	G	456	46.812	-17.943	83.354	1.00	24.43	C
ATOM	1999	C	ARG	G	456	47.642	-16.983	82.497	1.00	25.31	C
ATOM	2000	O	ARG	G	456	47.496	-16.940	81.270	1.00	25.02	O
ATOM	2001	CB	ARG	G	456	47.492	-19.307	83.356	1.00	24.98	C
ATOM	2002	CG	ARG	G	456	47.524	-19.973	81.992	1.00	27.29	C
ATOM	2003	CD	ARG	G	456	48.361	-21.238	81.995	1.00	26.58	C
ATOM	2004	NE	ARG	G	456	49.779	-20.977	82.237	1.00	26.43	N
ATOM	2005	CZ	ARG	G	456	50.761	-21.347	81.421	1.00	26.92	C
ATOM	2006	NH1	ARG	G	456	50.484	-22.002	80.306	1.00	29.13	N
ATOM	2007	NH2	ARG	G	456	52.018	-21.074	81.722	1.00	27.21	N
ATOM	2008	N	ASP	G	457	48.516	-16.221	83.152	1.00	26.11	N
ATOM	2009	CA	ASP	G	457	49.399	-15.289	82.456	1.00	27.22	C
ATOM	2010	C	ASP	G	457	50.363	-16.131	81.632	1.00	29.84	C
ATOM	2011	O	ASP	G	457	50.728	-17.246	82.031	1.00	30.22	O
ATOM	2012	CB	ASP	G	457	50.182	-14.417	83.453	1.00	24.42	C
ATOM	2013	CG	ASP	G	457	49.398	-13.195	83.925	1.00	20.39	C
ATOM	2014	OD1	ASP	G	457	48.176	-13.116	83.694	1.00	17.81	O
ATOM	2015	OD2	ASP	G	457	50.008	-12.292	84.529	1.00	17.85	O
ATOM	2016	N	GLY	G	458	50.766	-15.613	80.479	1.00	32.53	N
ATOM	2017	CA	GLY	G	458	51.676	-16.358	79.626	1.00	34.72	C
ATOM	2018	C	GLY	G	458	53.059	-15.760	79.495	1.00	35.98	C
ATOM	2019	O	GLY	G	458	53.524	-15.041	80.382	1.00	35.17	O
ATOM	2020	N	GLY	G	459	53.729	-16.104	78.397	1.00	37.74	N
ATOM	2021	CA	GLY	G	459	55.066	-15.602	78.135	1.00	42.30	C

FIG. 53-37

ATOM	2023	O	GLY G 459	57.194	-15.483	79.223	1.00	45.22	O
ATOM	2024	N	ASN G 460	55.684	-16.966	80.026	1.00	48.72	N
ATOM	2025	CA	ASN G 460	56.513	-17.465	81.120	1.00	50.85	C
ATOM	2026	C	ASN G 460	56.283	-18.974	81.242	1.00	50.87	C
ATOM	2027	O	ASN G 460	56.306	-19.544	82.334	1.00	50.15	O
ATOM	2028	CB	ASN G 460	56.107	-16.757	82.419	1.00	52.45	C
ATOM	2029	CG	ASN G 460	57.030	-17.076	83.573	1.00	54.62	C
ATOM	2030	OD1	ASN G 460	58.097	-16.475	83.716	1.00	56.03	O
ATOM	2031	ND2	ASN G 460	56.636	-18.036	84.397	1.00	54.44	N
ATOM	2032	N	SER G 461	56.092	-19.619	80.096	1.00	51.32	N
ATOM	2033	CA	SER G 461	55.829	-21.051	80.038	1.00	51.66	C
ATOM	2034	C	SER G 461	56.853	-21.875	80.820	1.00	51.52	C
ATOM	2035	O	SER G 461	58.055	-21.631	80.733	1.00	51.69	O
ATOM	2036	CB	SER G 461	55.782	-21.502	78.570	1.00	52.14	C
ATOM	2037	OG	SER G 461	55.295	-22.825	78.424	1.00	50.74	O
ATOM	2038	N	ASN G 462	56.347	-22.778	81.658	1.00	51.54	N
ATOM	2039	CA	ASN G 462	57.160	-23.698	82.467	1.00	51.71	C
ATOM	2040	C	ASN G 462	58.189	-23.092	83.431	1.00	51.30	C
ATOM	2041	O	ASN G 462	58.935	-23.836	84.074	1.00	51.47	O
ATOM	2042	CB	ASN G 462	57.890	-24.706	81.567	1.00	51.79	C
ATOM	2043	CG	ASN G 462	57.045	-25.198	80.406	1.00	51.91	C
ATOM	2044	OD1	ASN G 462	56.188	-26.072	80.573	1.00	52.36	O
ATOM	2045	ND2	ASN G 462	57.299	-24.652	79.219	1.00	50.59	N
ATOM	2046	N	ASN G 463	58.238	-21.766	83.537	1.00	50.19	N
ATOM	2047	CA	ASN G 463	59.200	-21.093	84.422	1.00	47.89	C
ATOM	2048	C	ASN G 463	58.755	-21.152	85.896	1.00	45.80	C
ATOM	2049	O	ASN G 463	57.704	-21.710	86.207	1.00	46.07	O
ATOM	2050	CB	ASN G 463	59.409	-19.645	83.955	1.00	47.92	C
ATOM	2051	CG	ASN G 463	60.579	-18.960	84.642	1.00	47.51	C
ATOM	2052	OD1	ASN G 463	61.518	-19.608	85.098	1.00	46.84	O
ATOM	2053	ND2	ASN G 463	60.518	-17.638	84.727	1.00	47.03	N
ATOM	2054	N	GLU G 464	59.530	-20.553	86.794	1.00	43.03	N
ATOM	2055	CA	GLU G 464	59.227	-20.577	88.224	1.00	40.21	C
ATOM	2056	C	GLU G 464	57.888	-20.097	88.778	1.00	37.07	C
ATOM	2057	O	GLU G 464	57.454	-20.582	89.825	1.00	37.50	O
ATOM	2058	CB	GLU G 464	60.374	-19.953	89.021	1.00	40.87	C
ATOM	2059	CG	GLU G 464	61.668	-20.741	88.900	1.00	41.67	C
ATOM	2060	CD	GLU G 464	61.450	-22.230	89.078	1.00	41.03	C
ATOM	2061	OE1	GLU G 464	61.274	-22.671	90.235	1.00	42.50	O
ATOM	2062	OE2	GLU G 464	61.423	-22.952	88.058	1.00	39.27	O
ATOM	2063	N	SER G 465	57.216	-19.175	88.102	1.00	32.54	N
ATOM	2064	CA	SER G 465	55.935	-18.693	88.618	1.00	29.12	C
ATOM	2065	C	SER G 465	54.817	-18.762	87.595	1.00	26.81	C
ATOM	2066	O	SER G 465	55.070	-18.752	86.395	1.00	27.05	O
ATOM	2067	CB	SER G 465	56.060	-17.259	89.136	1.00	28.35	C
ATOM	2068	OG	SER G 465	56.650	-17.216	90.426	1.00	27.82	O
ATOM	2069	N	GLU G 466	53.582	-18.846	88.076	1.00	24.12	N
ATOM	2070	CA	GLU G 466	52.421	-18.895	87.202	1.00	23.43	C
ATOM	2071	C	GLU G 466	51.353	-18.009	87.817	1.00	22.73	C
ATOM	2072	O	GLU G 466	50.918	-18.254	88.935	1.00	22.13	O
ATOM	2073	CB	GLU G 466	51.883	-20.320	87.071	1.00	25.08	C
ATOM	2074	CG	GLU G 466	52.819	-21.325	86.405	1.00	27.43	C
ATOM	2075	CD	GLU G 466	53.174	-20.957	84.981	1.00	27.92	C
ATOM	2076	OE1	GLU G 466	52.354	-20.282	84.319	1.00	27.68	O
ATOM	2077	OE2	GLU G 466	54.269	-21.363	84.522	1.00	27.89	O
ATOM	2078	N	ILE G 467	50.970	-16.954	87.104	1.00	21.51	N
ATOM	2079	CA	ILE G 467	49.956	-16.027	87.581	1.00	19.59	C
ATOM	2080	C	ILE G 467	48.600	-16.506	87.084	1.00	18.09	C
ATOM	2081	O	ILE G 467	48.475	-16.904	85.925	1.00	19.05	O
ATOM	2082	CB	ILE G 467	50.195	-14.589	87.053	1.00	20.01	C
ATOM	2083	CG1	ILE G 467	51.511	-14.014	87.596	1.00	21.88	C
ATOM	2084	CG2	ILE G 467	49.039	-13.678	87.465	1.00	18.52	C
ATOM	2085	CD1	ILE G 467	52.770	-14.461	86.849	1.00	23.23	C
ATOM	2086	N	PHE G 468	47.593	-16.469	87.957	1.00	15.14	N
ATOM	2087	CA	PHE G 468	46.239	-16.888	87.605	1.00	11.77	C
ATOM	2088	C	PHE G 468	45.268	-15.798	87.991	1.00	11.15	C
ATOM	2089	O	PHE G 468	45.252	-15.355	89.141	1.00	11.64	O
ATOM	2090	CB	PHE G 468	45.855	-18.167	88.343	1.00	9.01	C
ATOM	2091	CG	PHE G 468	46.752	-19.319	88.044	1.00	8.15	C
ATOM	2092	CD1	PHE G 468	47.923	-19.499	88.766	1.00	4.60	C

FIG. 53-38

ATOM	2094	CE1	PHE	G	468	48.785	-20.535	88.460	1.00	5.10	C
ATOM	2095	CE2	PHE	G	468	47.318	-21.242	86.695	1.00	6.47	C
ATOM	2096	CZ	PHE	G	468	48.487	-21.406	87.424	1.00	5.03	C
ATOM	2097	N	ARG	G	469	44.448	-15.376	87.043	1.00	10.23	N
ATOM	2098	CA	ARG	G	469	43.470	-14.326	87.311	1.00	10.26	C
ATOM	2099	C	ARG	G	469	42.069	-14.862	87.094	1.00	8.75	C
ATOM	2100	O	ARG	G	469	41.874	-15.834	86.377	1.00	9.27	O
ATOM	2101	CB	ARG	G	469	43.691	-13.141	86.365	1.00	8.59	C
ATOM	2102	CG	ARG	G	469	45.117	-12.665	86.292	1.00	8.69	C
ATOM	2103	CD	ARG	G	469	45.258	-11.600	85.246	1.00	10.54	C
ATOM	2104	NE	ARG	G	469	46.654	-11.230	85.027	1.00	12.67	N
ATOM	2105	CZ	ARG	G	469	47.195	-10.061	85.360	1.00	11.60	C
ATOM	2106	NH1	ARG	G	469	46.466	-9.122	85.953	1.00	9.15	N
ATOM	2107	NH2	ARG	G	469	48.462	-9.829	85.061	1.00	13.57	N
ATOM	2108	N	PRO	G	470	41.076	-14.233	87.721	1.00	8.09	N
ATOM	2109	CA	PRO	G	470	39.682	-14.644	87.584	1.00	9.26	C
ATOM	2110	C	PRO	G	470	39.227	-14.487	86.129	1.00	9.58	C
ATOM	2111	O	PRO	G	470	39.766	-13.656	85.379	1.00	10.54	O
ATOM	2112	CB	PRO	G	470	38.956	-13.658	88.490	1.00	11.72	C
ATOM	2113	CG	PRO	G	470	39.816	-12.447	88.418	1.00	10.44	C
ATOM	2114	CD	PRO	G	470	41.178	-13.047	88.579	1.00	9.29	C
ATOM	2115	N	GLY	G	471	38.197	-15.233	85.749	1.00	6.90	N
ATOM	2116	CA	GLY	G	471	37.719	-15.171	84.382	1.00	3.74	C
ATOM	2117	C	GLY	G	471	36.224	-15.326	84.324	1.00	3.27	C
ATOM	2118	O	GLY	G	471	35.517	-15.032	85.280	1.00	3.93	O
ATOM	2119	N	GLY	G	472	35.742	-15.828	83.203	1.00	4.03	N
ATOM	2120	CA	GLY	G	472	34.317	-16.007	83.032	1.00	5.04	C
ATOM	2121	C	GLY	G	472	33.908	-15.225	81.807	1.00	5.06	C
ATOM	2122	O	GLY	G	472	34.739	-14.576	81.167	1.00	5.90	O
ATOM	2123	N	GLY	G	473	32.629	-15.267	81.481	1.00	5.75	N
ATOM	2124	CA	GLY	G	473	32.158	-14.548	80.312	1.00	8.01	C
ATOM	2125	C	GLY	G	473	31.368	-15.484	79.429	1.00	8.42	C
ATOM	2126	O	GLY	G	473	30.239	-15.171	79.032	1.00	8.69	O
ATOM	2127	N	ASP	G	474	31.958	-16.630	79.109	1.00	8.01	N
ATOM	2128	CA	ASP	G	474	31.248	-17.588	78.287	1.00	10.05	C
ATOM	2129	C	ASP	G	474	30.379	-18.349	79.262	1.00	10.61	C
ATOM	2130	O	ASP	G	474	30.880	-19.102	80.092	1.00	11.51	O
ATOM	2131	CB	ASP	G	474	32.211	-18.536	77.569	1.00	12.12	C
ATOM	2132	CG	ASP	G	474	31.530	-19.324	76.444	1.00	15.87	C
ATOM	2133	OD1	ASP	G	474	30.274	-19.380	76.408	1.00	15.73	O
ATOM	2134	OD2	ASP	G	474	32.248	-19.870	75.573	1.00	17.45	O
ATOM	2135	N	MET	G	475	29.082	-18.087	79.236	1.00	10.97	N
ATOM	2136	CA	MET	G	475	28.185	-18.779	80.148	1.00	12.17	C
ATOM	2137	C	MET	G	475	28.191	-20.282	79.883	1.00	11.60	C
ATOM	2138	O	MET	G	475	27.747	-21.067	80.726	1.00	12.20	O
ATOM	2139	CB	MET	G	475	26.774	-18.209	80.056	1.00	14.44	C
ATOM	2140	CG	MET	G	475	26.231	-17.736	81.395	1.00	15.72	C
ATOM	2141	SD	MET	G	475	27.411	-16.723	82.311	1.00	17.42	S
ATOM	2142	CE	MET	G	475	27.326	-15.188	81.444	1.00	16.54	C
ATOM	2143	N	ARG	G	476	28.716	-20.684	78.725	1.00	11.20	N
ATOM	2144	CA	ARG	G	476	28.808	-22.097	78.377	1.00	8.61	C
ATOM	2145	C	ARG	G	476	29.737	-22.729	79.392	1.00	7.65	C
ATOM	2146	O	ARG	G	476	29.467	-23.809	79.902	1.00	8.65	O
ATOM	2147	CB	ARG	G	476	29.375	-22.285	76.970	1.00	8.85	C
ATOM	2148	CG	ARG	G	476	28.434	-21.940	75.854	1.00	7.46	C
ATOM	2149	CD	ARG	G	476	29.093	-22.121	74.504	1.00	10.82	C
ATOM	2150	NE	ARG	G	476	28.198	-21.721	73.417	1.00	16.50	N
ATOM	2151	CZ	ARG	G	476	27.968	-20.457	73.051	1.00	18.86	C
ATOM	2152	NH1	ARG	G	476	28.580	-19.452	73.682	1.00	19.84	N
ATOM	2153	NH2	ARG	G	476	27.090	-20.195	72.085	1.00	18.06	N
ATOM	2154	N	ASP	G	477	30.809	-22.024	79.730	1.00	7.09	N
ATOM	2155	CA	ASP	G	477	31.766	-22.520	80.710	1.00	7.45	C
ATOM	2156	C	ASP	G	477	31.134	-22.709	82.105	1.00	7.05	C
ATOM	2157	O	ASP	G	477	31.748	-23.292	82.999	1.00	8.82	O
ATOM	2158	CB	ASP	G	477	32.970	-21.583	80.787	1.00	7.33	C
ATOM	2159	CG	ASP	G	477	33.951	-21.790	79.650	1.00	9.77	C
ATOM	2160	OD1	ASP	G	477	33.775	-22.741	78.852	1.00	11.46	O
ATOM	2161	OD2	ASP	G	477	34.928	-21.010	79.565	1.00	10.97	O
ATOM	2162	N	ASN	G	478	29.914	-22.207	82.276	1.00	6.21	N
ATOM	2163	CA	ASN	G	478	29.156	-22.313	83.522	1.00	7.08	C

FIG. 53-39

ATOM	2165	O	ASN	G	478	28.013	-24.195	84.510	1.00	8.61	O
ATOM	2166	CB	ASN	G	478	28.226	-21.106	83.679	1.00	6.30	C
ATOM	2167	CG	ASN	G	478	28.946	-19.851	84.155	1.00	6.66	C
ATOM	2168	OD1	ASN	G	478	28.388	-19.083	84.941	1.00	6.95	O
ATOM	2169	ND2	ASN	G	478	30.181	-19.638	83.692	1.00	2.00	N
ATOM	2170	N	TRP	G	479	27.822	-23.918	82.288	1.00	10.60	N
ATOM	2171	CA	TRP	G	479	27.021	-25.117	82.112	1.00	10.15	C
ATOM	2172	C	TRP	G	479	27.982	-26.318	82.084	1.00	10.73	C
ATOM	2173	O	TRP	G	479	27.695	-27.380	82.620	1.00	10.51	O
ATOM	2174	CB	TRP	G	479	26.241	-25.049	80.799	1.00	9.36	C
ATOM	2175	CG	TRP	G	479	25.553	-23.727	80.471	1.00	9.36	C
ATOM	2176	CD1	TRP	G	479	25.260	-23.253	79.217	1.00	8.73	C
ATOM	2177	CD2	TRP	G	479	25.058	-22.734	81.390	1.00	10.20	C
ATOM	2178	NE1	TRP	G	479	24.622	-22.041	79.300	1.00	8.27	N
ATOM	2179	CE2	TRP	G	479	24.481	-21.698	80.617	1.00	9.64	C
ATOM	2180	CE3	TRP	G	479	25.043	-22.618	82.789	1.00	8.56	C
ATOM	2181	CZ2	TRP	G	479	23.897	-20.566	81.197	1.00	9.67	C
ATOM	2182	CZ3	TRP	G	479	24.461	-21.488	83.362	1.00	6.16	C
ATOM	2183	CH2	TRP	G	479	23.896	-20.481	82.566	1.00	5.85	C
ATOM	2184	N	ARG	G	480	29.147	-26.117	81.484	1.00	12.12	N
ATOM	2185	CA	ARG	G	480	30.182	-27.140	81.354	1.00	12.92	C
ATOM	2186	C	ARG	G	480	30.630	-27.739	82.686	1.00	11.60	C
ATOM	2187	O	ARG	G	480	30.971	-28.916	82.753	1.00	12.61	O
ATOM	2188	CB	ARG	G	480	31.386	-26.537	80.631	1.00	16.02	C
ATOM	2189	CG	ARG	G	480	32.292	-27.541	79.958	1.00	20.91	C
ATOM	2190	CD	ARG	G	480	33.048	-26.879	78.815	1.00	23.41	C
ATOM	2191	NE	ARG	G	480	32.155	-26.451	77.746	1.00	27.66	N
ATOM	2192	CZ	ARG	G	480	32.484	-25.573	76.800	1.00	30.70	C
ATOM	2193	NH1	ARG	G	480	33.691	-25.022	76.792	1.00	33.79	N
ATOM	2194	NH2	ARG	G	480	31.604	-25.258	75.852	1.00	32.11	N
ATOM	2195	N	SER	G	481	30.640	-26.926	83.738	1.00	10.12	N
ATOM	2196	CA	SER	G	481	31.049	-27.368	85.069	1.00	8.15	C
ATOM	2197	C	SER	G	481	30.074	-28.352	85.710	1.00	9.80	C
ATOM	2198	O	SER	G	481	30.440	-29.100	86.620	1.00	10.81	O
ATOM	2199	CB	SER	G	481	31.212	-26.154	85.983	1.00	7.90	C
ATOM	2200	OG	SER	G	481	30.037	-25.365	86.021	1.00	3.17	O
ATOM	2201	N	GLU	G	482	28.825	-28.311	85.262	1.00	11.73	N
ATOM	2202	CA	GLU	G	482	27.767	-29.187	85.764	1.00	13.27	C
ATOM	2203	C	GLU	G	482	27.511	-30.380	84.841	1.00	11.63	C
ATOM	2204	O	GLU	G	482	27.159	-31.467	85.295	1.00	11.49	O
ATOM	2205	CB	GLU	G	482	26.465	-28.395	85.923	1.00	15.44	C
ATOM	2206	CG	GLU	G	482	26.389	-27.534	87.168	1.00	18.18	C
ATOM	2207	CD	GLU	G	482	26.027	-28.317	88.421	1.00	20.60	C
ATOM	2208	OE1	GLU	G	482	26.223	-29.552	88.450	1.00	22.73	O
ATOM	2209	OE2	GLU	G	482	25.543	-27.694	89.389	1.00	19.58	O
ATOM	2210	N	LEU	G	483	27.707	-30.169	83.547	1.00	10.75	N
ATOM	2211	CA	LEU	G	483	27.473	-31.197	82.540	1.00	12.96	C
ATOM	2212	C	LEU	G	483	28.697	-32.002	82.100	1.00	14.52	C
ATOM	2213	O	LEU	G	483	28.565	-32.925	81.310	1.00	15.31	O
ATOM	2214	CB	LEU	G	483	26.822	-30.562	81.308	1.00	11.55	C
ATOM	2215	CG	LEU	G	483	25.442	-29.946	81.546	1.00	13.17	C
ATOM	2216	CD1	LEU	G	483	25.059	-29.037	80.396	1.00	13.84	C
ATOM	2217	CD2	LEU	G	483	24.413	-31.042	81.734	1.00	14.83	C
ATOM	2218	N	TYR	G	484	29.871	-31.692	82.637	1.00	16.23	N
ATOM	2219	CA	TYR	G	484	31.097	-32.394	82.261	1.00	17.00	C
ATOM	2220	C	TYR	G	484	30.984	-33.923	82.234	1.00	17.95	C
ATOM	2221	O	TYR	G	484	31.395	-34.571	81.274	1.00	20.37	O
ATOM	2222	CB	TYR	G	484	32.254	-31.985	83.187	1.00	15.95	C
ATOM	2223	CG	TYR	G	484	32.069	-32.445	84.615	1.00	15.50	C
ATOM	2224	CD1	TYR	G	484	31.191	-31.785	85.470	1.00	15.36	C
ATOM	2225	CD2	TYR	G	484	32.720	-33.580	85.091	1.00	13.89	C
ATOM	2226	CE1	TYR	G	484	30.954	-32.245	86.757	1.00	14.83	C
ATOM	2227	CE2	TYR	G	484	32.494	-34.047	86.375	1.00	14.19	C
ATOM	2228	CZ	TYR	G	484	31.608	-33.378	87.204	1.00	14.52	C
ATOM	2229	OH	TYR	G	484	31.363	-33.858	88.469	1.00	15.36	O
ATOM	2230	N	LYS	G	485	30.375	-34.485	83.268	1.00	17.99	N
ATOM	2231	CA	LYS	G	485	30.242	-35.929	83.409	1.00	17.32	C
ATOM	2232	C	LYS	G	485	29.132	-36.579	82.592	1.00	17.71	C
ATOM	2233	O	LYS	G	485	28.823	-37.755	82.805	1.00	17.90	O
ATOM	2234	CB	LYS	G	485	30.030	-36.263	84.886	1.00	17.90	C

FIG. 53-40

ATOM	2236	CD	LYS	G	485	28.630	-35.946	86.953	1.00	23.44	C
ATOM	2237	CE	LYS	G	485	27.333	-35.384	87.511	1.00	24.11	C
ATOM	2238	NZ	LYS	G	485	27.363	-35.232	88.997	1.00	27.95	N
ATOM	2239	N	TYR	G	486	28.543	-35.841	81.659	1.00	17.11	N
ATOM	2240	CA	TYR	G	486	27.447	-36.366	80.857	1.00	17.88	C
ATOM	2241	C	TYR	G	486	27.750	-36.388	79.377	1.00	19.48	C
ATOM	2242	O	TYR	G	486	28.700	-35.750	78.925	1.00	20.91	O
ATOM	2243	CB	TYR	G	486	26.196	-35.536	81.103	1.00	17.29	C
ATOM	2244	CG	TYR	G	486	25.733	-35.593	82.534	1.00	17.41	C
ATOM	2245	CD1	TYR	G	486	25.207	-36.770	83.058	1.00	17.47	C
ATOM	2246	CD2	TYR	G	486	25.823	-34.479	83.368	1.00	17.17	C
ATOM	2247	CE1	TYR	G	486	24.798	-36.844	84.371	1.00	17.71	C
ATOM	2248	CE2	TYR	G	486	25.412	-34.545	84.688	1.00	17.80	C
ATOM	2249	CZ	TYR	G	486	24.890	-35.733	85.182	1.00	16.96	C
ATOM	2250	OH	TYR	G	486	24.426	-35.824	86.474	1.00	18.30	O
ATOM	2251	N	LYS	G	487	26.956	-37.153	78.633	1.00	21.02	N
ATOM	2252	CA	LYS	G	487	27.107	-37.270	77.183	1.00	22.41	C
ATOM	2253	C	LYS	G	487	25.876	-37.937	76.587	1.00	22.55	C
ATOM	2254	O	LYS	G	487	25.287	-38.846	77.186	1.00	23.00	O
ATOM	2255	CB	LYS	G	487	28.355	-38.079	76.802	1.00	22.79	C
ATOM	2256	CG	LYS	G	487	28.218	-39.580	76.982	1.00	24.83	C
ATOM	2257	CD	LYS	G	487	29.353	-40.349	76.297	1.00	26.69	C
ATOM	2258	CE	LYS	G	487	29.241	-40.309	74.780	1.00	27.37	C
ATOM	2259	NZ	LYS	G	487	30.397	-40.984	74.131	1.00	27.40	N
ATOM	2260	N	VAL	G	488	25.507	-37.499	75.393	1.00	22.37	N
ATOM	2261	CA	VAL	G	488	24.352	-38.047	74.705	1.00	21.76	C
ATOM	2262	C	VAL	G	488	24.815	-39.007	73.602	1.00	22.79	C
ATOM	2263	O	VAL	G	488	25.655	-38.660	72.765	1.00	22.14	O
ATOM	2264	CB	VAL	G	488	23.444	-36.889	74.179	1.00	19.90	C
ATOM	2265	CG1	VAL	G	488	23.652	-36.617	72.700	1.00	19.39	C
ATOM	2266	CG2	VAL	G	488	22.007	-37.165	74.506	1.00	18.16	C
ATOM	2267	N	VAL	G	489	24.348	-40.245	73.673	1.00	24.24	N
ATOM	2268	CA	VAL	G	489	24.711	-41.265	72.687	1.00	26.29	C
ATOM	2269	C	VAL	G	489	23.457	-41.685	71.927	1.00	28.45	C
ATOM	2270	O	VAL	G	489	22.369	-41.759	72.504	1.00	29.28	O
ATOM	2271	CB	VAL	G	489	25.363	-42.514	73.366	1.00	25.74	C
ATOM	2272	CG1	VAL	G	489	24.332	-43.315	74.152	1.00	22.14	C
ATOM	2273	CG2	VAL	G	489	26.054	-43.389	72.331	1.00	26.00	C
ATOM	2274	N	LYS	G	490	23.588	-41.927	70.629	1.00	29.96	N
ATOM	2275	CA	LYS	G	490	22.431	-42.332	69.847	1.00	31.93	C
ATOM	2276	C	LYS	G	490	22.016	-43.753	70.218	1.00	34.03	C
ATOM	2277	O	LYS	G	490	22.850	-44.658	70.278	1.00	34.54	O
ATOM	2278	CB	LYS	G	490	22.704	-42.201	68.349	1.00	31.93	C
ATOM	2279	CG	LYS	G	490	21.465	-41.801	67.567	1.00	35.32	C
ATOM	2280	CD	LYS	G	490	21.785	-41.220	66.192	1.00	37.39	C
ATOM	2281	CE	LYS	G	490	20.529	-40.639	65.533	1.00	37.54	C
ATOM	2282	NZ	LYS	G	490	20.748	-40.207	64.118	1.00	38.65	N
ATOM	2283	N	ILE	G	491	20.734	-43.906	70.545	1.00	36.33	N
ATOM	2284	CA	ILE	G	491	20.129	-45.181	70.930	1.00	37.72	C
ATOM	2285	C	ILE	G	491	19.118	-45.588	69.858	1.00	39.67	C
ATOM	2286	O	ILE	G	491	18.473	-44.723	69.255	1.00	39.78	O
ATOM	2287	CB	ILE	G	491	19.406	-45.038	72.297	1.00	36.36	C
ATOM	2288	CG1	ILE	G	491	20.305	-45.522	73.430	1.00	36.68	C
ATOM	2289	CG2	ILE	G	491	18.075	-45.773	72.304	1.00	36.36	C
ATOM	2290	CD1	ILE	G	491	20.469	-47.033	73.500	1.00	38.02	C
ATOM	2291	N	GLU	G	492	19.004	-46.891	69.601	1.00	41.78	N
ATOM	2292	CA	GLU	G	492	18.060	-47.413	68.611	1.00	43.82	C
ATOM	2293	C	GLU	G	492	16.694	-47.697	69.252	1.00	45.10	C
ATOM	2294	O	GLU	G	492	15.761	-46.903	69.003	1.00	45.64	O
ATOM	2295	CB	GLU	G	492	18.615	-48.676	67.940	1.00	44.12	C
ATOM	2296	CG	GLU	G	492	19.829	-48.437	67.043	1.00	46.18	C
ATOM	2297	CD	GLU	G	492	20.457	-49.729	66.524	1.00	47.97	C
ATOM	2298	OE1	GLU	G	492	19.897	-50.348	65.588	1.00	47.56	O
ATOM	2299	OE2	GLU	G	492	21.529	-50.112	67.042	1.00	49.02	O
ATOM	2300	OXT	GLU	G	492	16.573	-48.673	70.027	1.00	45.10	O
TER	2301		GLU	G	492						
HETATM	2302	C1	NAG	G	697	20.555	-6.134	59.155	1.00	59.64	C
HETATM	2303	C2	NAG	G	697	19.931	-7.521	59.386	1.00	60.12	C
HETATM	2304	C3	NAG	G	697	20.278	-8.417	58.201	1.00	59.51	C
HETATM	2305	C4	NAG	G	697	19.721	-7.772	56.934	1.00	59.36	C

FIG. 53-41

HETATM	2307	C6	NAG	G 697	19.872	-5.633	55.538	1.00	60.21	C
HETATM	2308	C7	NAG	G 697	19.627	-8.793	61.463	1.00	60.60	C
HETATM	2309	C8	NAG	G 697	20.341	-9.325	62.699	1.00	59.35	C
HETATM	2310	N2	NAG	G 697	20.413	-8.118	60.621	1.00	61.24	N
HETATM	2311	O3	NAG	G 697	19.735	-9.718	58.380	1.00	58.83	O
HETATM	2312	O4	NAG	G 697	20.000	-8.588	55.801	1.00	59.07	O
HETATM	2313	O5	NAG	G 697	20.074	-5.567	57.924	1.00	59.41	O
HETATM	2314	O6	NAG	G 697	18.475	-5.375	55.596	1.00	60.26	O
HETATM	2315	O7	NAG	G 697	18.419	-8.955	61.273	1.00	59.25	O
HETATM	2316	C1	NAG	G 734	42.125	-35.659	83.656	1.00	51.27	C
HETATM	2317	C2	NAG	G 734	43.126	-36.498	84.440	1.00	53.64	C
HETATM	2318	C3	NAG	G 734	44.520	-35.939	84.253	1.00	53.54	C
HETATM	2319	C4	NAG	G 734	44.872	-35.991	82.769	1.00	52.32	C
HETATM	2320	C5	NAG	G 734	43.799	-35.348	81.871	1.00	51.37	C
HETATM	2321	C6	NAG	G 734	43.982	-35.804	80.439	1.00	49.85	C
HETATM	2322	C7	NAG	G 734	42.980	-35.689	86.776	1.00	56.96	C
HETATM	2323	C8	NAG	G 734	42.506	-36.091	88.159	1.00	57.39	C
HETATM	2324	N2	NAG	G 734	42.770	-36.622	85.845	1.00	56.31	N
HETATM	2325	O3	NAG	G 734	45.443	-36.720	84.998	1.00	54.53	O
HETATM	2326	O4	NAG	G 734	46.100	-35.311	82.562	1.00	50.81	O
HETATM	2327	O5	NAG	G 734	42.438	-35.744	82.248	1.00	50.85	O
HETATM	2328	O6	NAG	G 734	43.903	-37.244	80.404	1.00	49.02	O
HETATM	2329	O7	NAG	G 734	43.497	-34.596	86.541	1.00	57.93	O
HETATM	2330	C1	NAG	G 762	21.130	-19.832	94.879	1.00	20.43	C
HETATM	2331	C2	NAG	G 762	20.570	-19.167	96.139	1.00	22.02	C
HETATM	2332	C3	NAG	G 762	19.815	-17.879	95.806	1.00	23.32	C
HETATM	2333	C4	NAG	G 762	20.663	-16.976	94.933	1.00	24.20	C
HETATM	2334	C5	NAG	G 762	21.004	-17.767	93.674	1.00	24.06	C
HETATM	2335	C6	NAG	G 762	21.722	-16.987	92.586	1.00	21.85	C
HETATM	2336	C7	NAG	G 762	20.025	-21.017	97.650	1.00	28.11	C
HETATM	2337	C8	NAG	G 762	18.892	-21.870	98.197	1.00	28.87	C
HETATM	2338	N2	NAG	G 762	19.647	-20.087	96.780	1.00	25.44	N
HETATM	2339	O3	NAG	G 762	19.462	-17.195	96.994	1.00	23.53	O
HETATM	2340	O4	NAG	G 762	19.936	-15.797	94.615	1.00	25.52	O
HETATM	2341	O5	NAG	G 762	21.828	-18.891	94.044	1.00	24.01	O
HETATM	2342	O6	NAG	G 762	22.927	-16.416	93.070	1.00	22.76	O
HETATM	2343	O7	NAG	G 762	21.197	-21.180	97.986	1.00	29.82	O
HETATM	2344	C1	NAG	G 776	47.194	-26.706	72.904	1.00	29.03	C
HETATM	2345	C2	NAG	G 776	46.843	-26.624	71.420	1.00	28.27	C
HETATM	2346	C3	NAG	G 776	47.591	-25.464	70.776	1.00	29.77	C
HETATM	2347	C4	NAG	G 776	49.045	-25.425	71.270	1.00	30.66	C
HETATM	2348	C5	NAG	G 776	49.103	-25.289	72.793	1.00	30.69	C
HETATM	2349	C6	NAG	G 776	49.612	-23.936	73.245	1.00	31.96	C
HETATM	2350	C7	NAG	G 776	46.445	-28.953	70.822	1.00	26.40	C
HETATM	2351	C8	NAG	G 776	47.020	-30.157	70.096	1.00	27.26	C
HETATM	2352	N2	NAG	G 776	47.212	-27.870	70.777	1.00	26.77	N
HETATM	2353	O3	NAG	G 776	46.933	-24.240	71.085	1.00	32.45	O
HETATM	2354	O4	NAG	G 776	49.713	-26.616	70.881	1.00	31.22	O
HETATM	2355	O5	NAG	G 776	47.785	-25.480	73.353	1.00	30.33	O
HETATM	2356	O6	NAG	G 776	48.972	-22.885	72.538	1.00	34.50	O
HETATM	2357	O7	NAG	G 776	45.350	-28.970	71.381	1.00	25.78	O
HETATM	2358	C1	NAG	G 789	39.622	-31.812	99.985	1.00	33.09	C
HETATM	2359	C2	NAG	G 789	41.091	-31.595	100.379	1.00	35.79	C
HETATM	2360	C3	NAG	G 789	41.464	-32.456	101.583	1.00	38.23	C
HETATM	2361	C4	NAG	G 789	40.468	-32.287	102.728	1.00	38.02	C
HETATM	2362	C5	NAG	G 789	39.027	-32.466	102.205	1.00	37.00	C
HETATM	2363	C6	NAG	G 789	37.964	-32.196	103.263	1.00	36.92	C
HETATM	2364	C7	NAG	G 789	42.221	-31.188	98.239	1.00	38.71	C
HETATM	2365	C8	NAG	G 789	43.194	-31.796	97.241	1.00	38.54	C
HETATM	2366	N2	NAG	G 789	41.974	-31.962	99.288	1.00	36.82	N
HETATM	2367	O3	NAG	G 789	42.771	-32.119	102.028	1.00	40.34	O
HETATM	2368	O4	NAG	G 789	40.753	-33.260	103.734	1.00	36.57	O
HETATM	2369	O5	NAG	G 789	38.776	-31.559	101.110	1.00	33.56	O
HETATM	2370	O6	NAG	G 789	36.661	-32.387	102.737	1.00	34.73	O
HETATM	2371	O7	NAG	G 789	41.692	-30.092	98.076	1.00	40.67	O
HETATM	2372	C1	NAG	G 795	26.343	-15.597	105.566	1.00	33.85	C
HETATM	2373	C2	NAG	G 795	27.454	-15.427	106.588	1.00	34.59	C
HETATM	2374	C3	NAG	G 795	27.804	-16.830	107.085	1.00	33.53	C
HETATM	2375	C4	NAG	G 795	26.576	-17.377	107.789	1.00	34.67	C
HETATM	2376	C5	NAG	G 795	25.361	-17.390	106.844	1.00	35.20	C

FIG. 53-42

HETATM	2378	C7	NAG	G	795	29.721	-15.240	105.605	1.00	35.20	C
HETATM	2379	C8	NAG	G	795	30.722	-14.216	105.110	1.00	33.50	C
HETATM	2380	N2	NAG	G	795	28.585	-14.693	106.045	1.00	34.80	N
HETATM	2381	O3	NAG	G	795	28.901	-16.798	107.984	1.00	31.29	O
HETATM	2382	O4	NAG	G	795	26.838	-18.693	108.266	1.00	36.45	O
HETATM	2383	O5	NAG	G	795	25.164	-16.082	106.229	1.00	34.33	O
HETATM	2384	O6	NAG	G	795	22.929	-17.316	106.880	1.00	37.82	O
HETATM	2385	O7	NAG	G	795	29.948	-16.455	105.616	1.00	36.36	O
HETATM	2386	C1	NAG	G	832	28.226	-9.645	104.992	1.00	45.87	C
HETATM	2387	C2	NAG	G	832	27.974	-8.717	103.779	1.00	47.52	C
HETATM	2388	C3	NAG	G	832	26.672	-7.923	103.865	1.00	47.38	C
HETATM	2389	C4	NAG	G	832	25.536	-8.834	104.242	1.00	47.85	C
HETATM	2390	C5	NAG	G	832	25.893	-9.462	105.568	1.00	48.32	C
HETATM	2391	C6	NAG	G	832	24.771	-10.301	106.124	1.00	49.64	C
HETATM	2392	C7	NAG	G	832	29.433	-6.905	104.549	1.00	50.62	C
HETATM	2393	C8	NAG	G	832	30.638	-6.054	104.182	1.00	50.60	C
HETATM	2394	N2	NAG	G	832	29.086	-7.795	103.623	1.00	49.35	N
HETATM	2395	O3	NAG	G	832	26.389	-7.335	102.610	1.00	46.59	O
HETATM	2396	O4	NAG	G	832	24.339	-8.081	104.350	1.00	49.40	O
HETATM	2397	O5	NAG	G	832	27.025	-10.331	105.389	1.00	47.66	O
HETATM	2398	O6	NAG	G	832	24.829	-11.627	105.607	1.00	52.39	O
HETATM	2399	O7	NAG	G	832	28.806	-6.757	105.595	1.00	51.02	O
HETATM	2400	C1	NAG	G	839	45.384	-15.132	101.861	1.00	48.21	C
HETATM	2401	C2	NAG	G	839	45.794	-14.589	100.496	1.00	48.49	C
HETATM	2402	C3	NAG	G	839	44.600	-13.920	99.790	1.00	50.29	C
HETATM	2403	C4	NAG	G	839	43.333	-14.084	100.623	1.00	51.29	C
HETATM	2404	C5	NAG	G	839	43.588	-13.499	102.001	1.00	51.81	C
HETATM	2405	C6	NAG	G	839	42.436	-13.580	102.964	1.00	52.61	C
HETATM	2406	C7	NAG	G	839	46.867	-12.432	101.084	1.00	48.14	C
HETATM	2407	C8	NAG	G	839	48.204	-11.709	101.107	1.00	47.76	C
HETATM	2408	N2	NAG	G	839	46.931	-13.683	100.621	1.00	48.44	N
HETATM	2409	O3	NAG	G	839	44.391	-14.504	98.514	1.00	49.77	O
HETATM	2410	O4	NAG	G	839	42.266	-13.392	99.990	1.00	52.56	O
HETATM	2411	O5	NAG	G	839	44.717	-14.131	102.652	1.00	51.72	O
HETATM	2412	O6	NAG	G	839	42.786	-12.941	104.186	1.00	51.16	O
HETATM	2413	O7	NAG	G	839	45.824	-11.900	101.451	1.00	47.23	O
HETATM	2414	C1	NAG	G	886	38.263	-1.983	93.510	1.00	10.19	C
HETATM	2415	C2	NAG	G	886	39.603	-2.388	94.081	1.00	11.25	C
HETATM	2416	C3	NAG	G	886	40.644	-1.429	93.556	1.00	8.62	C
HETATM	2417	C4	NAG	G	886	40.684	-1.576	92.052	1.00	6.43	C
HETATM	2418	C5	NAG	G	886	39.309	-1.295	91.444	1.00	6.21	C
HETATM	2419	C6	NAG	G	886	39.275	-1.678	89.965	1.00	6.26	C
HETATM	2420	C7	NAG	G	886	39.359	-3.470	96.261	1.00	20.54	C
HETATM	2421	C8	NAG	G	886	39.345	-3.231	97.770	1.00	21.65	C
HETATM	2422	N2	NAG	G	886	39.557	-2.371	95.531	1.00	18.35	N
HETATM	2423	O3	NAG	G	886	41.918	-1.723	94.108	1.00	5.81	O
HETATM	2424	O4	NAG	G	886	41.632	-0.671	91.524	1.00	6.73	O
HETATM	2425	O5	NAG	G	886	38.286	-2.088	92.087	1.00	9.22	O
HETATM	2426	O6	NAG	G	886	37.970	-2.092	89.567	1.00	6.56	O
HETATM	2427	O7	NAG	G	886	39.224	-4.589	95.758	1.00	21.08	O
HETATM	2428	C1	NAG	G	892	46.184	-7.814	97.674	1.00	47.50	C
HETATM	2429	C2	NAG	G	892	45.528	-6.456	97.388	1.00	49.91	C
HETATM	2430	C3	NAG	G	892	44.626	-6.058	98.564	1.00	50.40	C
HETATM	2431	C4	NAG	G	892	43.661	-7.190	98.908	1.00	50.85	C
HETATM	2432	C5	NAG	G	892	44.446	-8.485	99.149	1.00	50.35	C
HETATM	2433	C6	NAG	G	892	43.620	-9.712	99.508	1.00	50.08	C
HETATM	2434	C7	NAG	G	892	46.349	-4.288	96.593	1.00	50.40	C
HETATM	2435	C8	NAG	G	892	47.573	-3.388	96.528	1.00	50.74	C
HETATM	2436	N2	NAG	G	892	46.560	-5.448	97.209	1.00	51.09	N
HETATM	2437	O3	NAG	G	892	43.880	-4.889	98.245	1.00	50.85	O
HETATM	2438	O4	NAG	G	892	42.920	-6.835	100.066	1.00	51.88	O
HETATM	2439	O5	NAG	G	892	45.198	-8.806	97.970	1.00	48.21	O
HETATM	2440	O6	NAG	G	892	42.430	-9.339	100.240	1.00	50.76	O
HETATM	2441	O7	NAG	G	892	45.259	-3.974	96.112	1.00	49.47	O
HETATM	2442	C1	NAG	G	948	25.295	-22.817	101.637	1.00	40.79	C
HETATM	2443	C2	NAG	G	948	24.518	-21.842	102.514	1.00	42.75	C
HETATM	2444	C3	NAG	G	948	24.415	-22.474	103.889	1.00	43.06	C
HETATM	2445	C4	NAG	G	948	23.648	-23.791	103.786	1.00	43.39	C
HETATM	2446	C5	NAG	G	948	24.232	-24.720	102.690	1.00	43.93	C
HETATM	2447	C6	NAG	G	948	23.250	-25.813	102.286	1.00	45.28	C

FIG. 53-43

HETATM	2449	C8	NAG	G	948	25.354	-18.157	102.738	1.00	45.91	C
HETATM	2450	N2	NAG	G	948	25.166	-20.546	102.603	1.00	44.95	N
HETATM	2451	O3	NAG	G	948	23.751	-21.592	104.775	1.00	41.16	O
HETATM	2452	O4	NAG	G	948	23.691	-24.450	105.045	1.00	44.20	O
HETATM	2453	O5	NAG	G	948	24.512	-23.997	101.459	1.00	43.27	O
HETATM	2454	O6	NAG	G	948	23.025	-26.747	103.362	1.00	45.76	O
HETATM	2455	O7	NAG	G	948	23.258	-19.349	102.552	1.00	45.87	O
HETATM	2456	C1	FUC	G	735	44.832	-37.819	79.533	1.00	49.89	C
HETATM	2457	C2	FUC	G	735	44.829	-39.335	79.729	1.00	50.29	C
HETATM	2458	C3	FUC	G	735	43.517	-39.947	79.245	1.00	49.55	C
HETATM	2459	C4	FUC	G	735	43.248	-39.510	77.810	1.00	49.76	C
HETATM	2460	C5	FUC	G	735	43.281	-37.985	77.709	1.00	51.03	C
HETATM	2461	C6	FUC	G	735	43.097	-37.486	76.286	1.00	50.15	C
HETATM	2462	O2	FUC	G	735	45.009	-39.644	81.103	1.00	51.19	O
HETATM	2463	O3	FUC	G	735	43.614	-41.363	79.303	1.00	47.91	O
HETATM	2464	O4	FUC	G	735	44.237	-40.067	76.958	1.00	48.59	O
HETATM	2465	O5	FUC	G	735	44.552	-37.492	78.179	1.00	50.30	O
HETATM	2466	C1	FUC	G	796	21.868	-18.232	106.944	1.00	39.18	C
HETATM	2467	C2	FUC	G	796	21.294	-18.306	108.369	1.00	39.82	C
HETATM	2468	C3	FUC	G	796	20.583	-16.994	108.738	1.00	40.37	C
HETATM	2469	C4	FUC	G	796	19.594	-16.548	107.660	1.00	41.30	C
HETATM	2470	C5	FUC	G	796	20.249	-16.583	106.284	1.00	41.12	C
HETATM	2471	C6	FUC	G	796	19.259	-16.299	105.170	1.00	41.28	C
HETATM	2472	O2	FUC	G	796	22.312	-18.587	109.324	1.00	36.01	O
HETATM	2473	O3	FUC	G	796	19.881	-17.154	109.963	1.00	39.31	O
HETATM	2474	O4	FUC	G	796	18.450	-17.385	107.680	1.00	41.95	O
HETATM	2475	O5	FUC	G	796	20.825	-17.887	106.043	1.00	40.79	O
HETATM	2476	C1	FUC	G	893	42.567	-9.258	101.642	1.00	50.80	C
HETATM	2477	C2	FUC	G	893	41.194	-9.514	102.274	1.00	50.38	C
HETATM	2478	C3	FUC	G	893	41.299	-10.170	103.654	1.00	49.12	C
HETATM	2479	C4	FUC	G	893	42.554	-9.716	104.378	1.00	49.68	C
HETATM	2480	C5	FUC	G	893	43.820	-10.036	103.564	1.00	50.81	C
HETATM	2481	C6	FUC	G	893	44.916	-8.991	103.707	1.00	50.38	C
HETATM	2482	O2	FUC	G	893	40.434	-10.355	101.418	1.00	50.40	O
HETATM	2483	O3	FUC	G	893	40.158	-9.815	104.427	1.00	46.21	O
HETATM	2484	O4	FUC	G	893	42.469	-8.324	104.642	1.00	50.60	O
HETATM	2485	O5	FUC	G	893	43.519	-10.180	102.153	1.00	50.37	O
HETATM	2486	C1	FUC	G	949	21.703	-26.733	103.844	1.00	48.86	C
HETATM	2487	C2	FUC	G	949	20.695	-27.189	102.761	1.00	49.59	C
HETATM	2488	C3	FUC	G	949	20.209	-28.600	103.072	1.00	50.21	C
HETATM	2489	C4	FUC	G	949	19.428	-28.569	104.380	1.00	50.60	C
HETATM	2490	C5	FUC	G	949	20.207	-27.783	105.445	1.00	51.10	C
HETATM	2491	C6	FUC	G	949	19.594	-26.439	105.805	1.00	50.80	C
HETATM	2492	O2	FUC	G	949	21.259	-27.160	101.459	1.00	49.78	O
HETATM	2493	O3	FUC	G	949	19.372	-29.064	102.021	1.00	50.49	O
HETATM	2494	O4	FUC	G	949	18.162	-27.963	104.155	1.00	49.46	O
HETATM	2495	O5	FUC	G	949	21.568	-27.546	105.009	1.00	49.90	O
ATOM	2496	N	LYS	C	1	52.519	-14.192	56.192	1.00	46.28	N
ATOM	2497	CA	LYS	C	1	52.501	-13.174	57.280	1.00	46.54	C
ATOM	2498	C	LYS	C	1	52.344	-11.780	56.675	1.00	45.07	C
ATOM	2499	O	LYS	C	1	53.179	-11.339	55.885	1.00	45.01	O
ATOM	2500	CB	LYS	C	1	53.779	-13.271	58.127	1.00	46.69	C
ATOM	2501	CG	LYS	C	1	54.092	-12.030	58.955	1.00	47.32	C
ATOM	2502	CD	LYS	C	1	55.232	-12.265	59.947	1.00	46.72	C
ATOM	2503	CE	LYS	C	1	56.361	-13.127	59.377	1.00	44.02	C
ATOM	2504	NZ	LYS	C	1	56.425	-14.429	60.099	1.00	42.44	N
ATOM	2505	N	LYS	C	2	51.240	-11.128	57.024	1.00	42.82	N
ATOM	2506	CA	LYS	C	2	50.914	-9.794	56.542	1.00	40.43	C
ATOM	2507	C	LYS	C	2	51.775	-8.746	57.238	1.00	38.15	C
ATOM	2508	O	LYS	C	2	52.171	-8.921	58.398	1.00	37.03	O
ATOM	2509	CB	LYS	C	2	49.436	-9.500	56.824	1.00	42.05	C
ATOM	2510	CG	LYS	C	2	48.531	-9.514	55.603	1.00	45.12	C
ATOM	2511	CD	LYS	C	2	48.547	-8.172	54.888	1.00	48.62	C
ATOM	2512	CE	LYS	C	2	48.042	-7.054	55.805	1.00	50.79	C
ATOM	2513	NZ	LYS	C	2	46.646	-7.283	56.307	1.00	52.67	N
ATOM	2514	N	VAL	C	3	52.078	-7.674	56.512	1.00	35.75	N
ATOM	2515	CA	VAL	C	3	52.865	-6.562	57.047	1.00	32.56	C
ATOM	2516	C	VAL	C	3	51.990	-5.307	57.081	1.00	29.97	C
ATOM	2517	O	VAL	C	3	51.403	-4.913	56.067	1.00	32.06	O
ATOM	2518	CB	VAL	C	3	54.123	-6.276	56.188	1.00	32.08	C

FIG. 53-44

ATOM	2520	CG2	VAL	C	3	54.979	-7.515	56.081	1.00	32.20	C
ATOM	2521	N	VAL	C	4	51.873	-4.705	58.253	1.00	26.84	N
ATOM	2522	CA	VAL	C	4	51.081	-3.499	58.422	1.00	24.56	C
ATOM	2523	C	VAL	C	4	51.964	-2.412	59.032	1.00	23.09	C
ATOM	2524	O	VAL	C	4	52.702	-2.657	59.991	1.00	23.17	O
ATOM	2525	CB	VAL	C	4	49.862	-3.754	59.335	1.00	25.14	C
ATOM	2526	CG1	VAL	C	4	49.174	-2.440	59.688	1.00	25.88	C
ATOM	2527	CG2	VAL	C	4	48.884	-4.696	58.653	1.00	24.55	C
ATOM	2528	N	LEU	C	5	51.930	-1.228	58.435	1.00	20.69	N
ATOM	2529	CA	LEU	C	5	52.713	-0.110	58.920	1.00	17.71	C
ATOM	2530	C	LEU	C	5	51.767	0.875	59.563	1.00	16.21	C
ATOM	2531	O	LEU	C	5	50.640	1.053	59.102	1.00	14.03	O
ATOM	2532	CB	LEU	C	5	53.452	0.571	57.771	1.00	19.17	C
ATOM	2533	CG	LEU	C	5	54.976	0.433	57.740	1.00	19.31	C
ATOM	2534	CD1	LEU	C	5	55.349	-1.015	57.430	1.00	20.41	C
ATOM	2535	CD2	LEU	C	5	55.560	1.376	56.692	1.00	17.06	C
ATOM	2536	N	GLY	C	6	52.237	1.502	60.635	1.00	16.84	N
ATOM	2537	CA	GLY	C	6	51.444	2.477	61.357	1.00	14.53	C
ATOM	2538	C	GLY	C	6	52.278	3.696	61.701	1.00	13.29	C
ATOM	2539	O	GLY	C	6	53.518	3.670	61.634	1.00	9.47	O
ATOM	2540	N	LYS	C	7	51.590	4.756	62.110	1.00	13.42	N
ATOM	2541	CA	LYS	C	7	52.228	6.017	62.456	1.00	14.70	C
ATOM	2542	C	LYS	C	7	52.227	6.231	63.966	1.00	15.10	C
ATOM	2543	O	LYS	C	7	51.268	5.875	64.644	1.00	15.26	O
ATOM	2544	CB	LYS	C	7	51.506	7.166	61.726	1.00	16.29	C
ATOM	2545	CG	LYS	C	7	51.575	7.042	60.191	1.00	17.07	C
ATOM	2546	CD	LYS	C	7	50.476	7.796	59.437	1.00	17.81	C
ATOM	2547	CE	LYS	C	7	50.659	9.310	59.449	1.00	20.57	C
ATOM	2548	NZ	LYS	C	7	50.313	9.923	60.770	1.00	28.17	N
ATOM	2549	N	LYS	C	8	53.329	6.755	64.499	1.00	17.20	N
ATOM	2550	CA	LYS	C	8	53.441	7.017	65.934	1.00	17.81	C
ATOM	2551	C	LYS	C	8	52.301	7.941	66.330	1.00	18.97	C
ATOM	2552	O	LYS	C	8	52.166	9.040	65.777	1.00	20.57	O
ATOM	2553	CB	LYS	C	8	54.782	7.686	66.265	1.00	16.85	C
ATOM	2554	CG	LYS	C	8	54.858	8.299	67.669	1.00	21.33	C
ATOM	2555	CD	LYS	C	8	56.179	9.042	67.918	1.00	25.64	C
ATOM	2556	CE	LYS	C	8	56.335	10.290	67.008	1.00	29.41	C
ATOM	2557	NZ	LYS	C	8	57.754	10.788	66.887	1.00	28.75	N
ATOM	2558	N	GLY	C	9	51.445	7.464	67.229	1.00	19.05	N
ATOM	2559	CA	GLY	C	9	50.330	8.268	67.696	1.00	17.56	C
ATOM	2560	C	GLY	C	9	48.969	7.980	67.102	1.00	17.59	C
ATOM	2561	O	GLY	C	9	47.958	8.239	67.756	1.00	16.57	O
ATOM	2562	N	ASP	C	10	48.923	7.437	65.888	1.00	19.01	N
ATOM	2563	CA	ASP	C	10	47.643	7.139	65.239	1.00	21.62	C
ATOM	2564	C	ASP	C	10	46.957	5.928	65.855	1.00	23.44	C
ATOM	2565	O	ASP	C	10	47.401	5.406	66.878	1.00	24.09	O
ATOM	2566	CB	ASP	C	10	47.824	6.914	63.730	1.00	22.83	C
ATOM	2567	CG	ASP	C	10	47.971	8.218	62.942	1.00	24.07	C
ATOM	2568	OD1	ASP	C	10	47.688	9.309	63.483	1.00	25.82	O
ATOM	2569	OD2	ASP	C	10	48.369	8.149	61.759	1.00	22.11	O
ATOM	2570	N	THR	C	11	45.879	5.479	65.217	1.00	25.01	N
ATOM	2571	CA	THR	C	11	45.106	4.328	65.679	1.00	25.73	C
ATOM	2572	C	THR	C	11	45.002	3.295	64.559	1.00	25.74	C
ATOM	2573	O	THR	C	11	44.371	3.541	63.526	1.00	27.41	O
ATOM	2574	CB	THR	C	11	43.690	4.769	66.127	1.00	25.46	C
ATOM	2575	OG1	THR	C	11	43.796	5.608	67.287	1.00	24.74	O
ATOM	2576	CG2	THR	C	11	42.827	3.573	66.460	1.00	25.70	C
ATOM	2577	N	VAL	C	12	45.634	2.148	64.759	1.00	25.59	N
ATOM	2578	CA	VAL	C	12	45.634	1.090	63.753	1.00	25.97	C
ATOM	2579	C	VAL	C	12	44.625	-0.028	64.043	1.00	26.00	C
ATOM	2580	O	VAL	C	12	44.258	-0.272	65.193	1.00	26.72	O
ATOM	2581	CB	VAL	C	12	47.063	0.485	63.592	1.00	24.36	C
ATOM	2582	CG1	VAL	C	12	47.418	-0.371	64.790	1.00	25.22	C
ATOM	2583	CG2	VAL	C	12	47.175	-0.312	62.312	1.00	23.23	C
ATOM	2584	N	GLU	C	13	44.154	-0.680	62.990	1.00	25.92	N
ATOM	2585	CA	GLU	C	13	43.220	-1.783	63.147	1.00	27.89	C
ATOM	2586	C	GLU	C	13	43.732	-3.000	62.387	1.00	28.19	C
ATOM	2587	O	GLU	C	13	43.845	-2.979	61.162	1.00	30.05	O
ATOM	2588	CB	GLU	C	13	41.816	-1.424	62.650	1.00	28.29	C
ATOM	2589	CG	GLU	C	13	40.854	-2.614	62.693	1.00	29.78	C

FIG. 53-45

ATOM	2591	OE1	GLU	C	13	38.709	-1.591	62.650	1.00	31.72	O
ATOM	2592	OE2	GLU	C	13	39.268	-2.846	60.934	1.00	30.92	O
ATOM	2593	N	LEU	C	14	44.122	-4.028	63.127	1.00	27.86	N
ATOM	2594	CA	LEU	C	14	44.607	-5.264	62.534	1.00	25.77	C
ATOM	2595	C	LEU	C	14	43.350	-6.099	62.310	1.00	25.26	C
ATOM	2596	O	LEU	C	14	42.456	-6.102	63.159	1.00	24.53	O
ATOM	2597	CB	LEU	C	14	45.582	-5.949	63.493	1.00	25.87	C
ATOM	2598	CG	LEU	C	14	46.783	-5.061	63.861	1.00	26.59	C
ATOM	2599	CD1	LEU	C	14	47.658	-5.719	64.905	1.00	26.29	C
ATOM	2600	CD2	LEU	C	14	47.592	-4.744	62.621	1.00	24.92	C
ATOM	2601	N	THR	C	15	43.274	-6.770	61.160	1.00	25.71	N
ATOM	2602	CA	THR	C	15	42.113	-7.583	60.774	1.00	24.95	C
ATOM	2603	C	THR	C	15	42.204	-9.088	61.074	1.00	24.16	C
ATOM	2604	O	THR	C	15	43.286	-9.686	61.056	1.00	22.82	O
ATOM	2605	CB	THR	C	15	41.802	-7.413	59.257	1.00	24.70	C
ATOM	2606	OG1	THR	C	15	42.537	-6.299	58.736	1.00	23.44	O
ATOM	2607	CG2	THR	C	15	40.314	-7.166	59.037	1.00	24.46	C
ATOM	2608	N	CYS	C	16	41.042	-9.690	61.317	1.00	23.58	N
ATOM	2609	CA	CYS	C	16	40.943	-11.117	61.596	1.00	24.66	C
ATOM	2610	C	CYS	C	16	39.517	-11.581	61.317	1.00	25.93	C
ATOM	2611	O	CYS	C	16	38.567	-11.126	61.969	1.00	23.82	O
ATOM	2612	CB	CYS	C	16	41.300	-11.415	63.046	1.00	24.59	C
ATOM	2613	SG	CYS	C	16	41.474	-13.182	63.435	1.00	22.70	S
ATOM	2614	N	THR	C	17	39.381	-12.482	60.346	1.00	28.46	N
ATOM	2615	CA	THR	C	17	38.082	-13.008	59.955	1.00	30.73	C
ATOM	2616	C	THR	C	17	38.059	-14.522	60.073	1.00	31.96	C
ATOM	2617	O	THR	C	17	38.757	-15.232	59.345	1.00	32.62	O
ATOM	2618	CB	THR	C	17	37.716	-12.576	58.519	1.00	31.47	C
ATOM	2619	OG1	THR	C	17	37.644	-11.143	58.458	1.00	32.79	O
ATOM	2620	CG2	THR	C	17	36.376	-13.154	58.109	1.00	31.32	C
ATOM	2621	N	ALA	C	18	37.258	-15.005	61.016	1.00	34.59	N
ATOM	2622	CA	ALA	C	18	37.105	-16.432	61.271	1.00	37.71	C
ATOM	2623	C	ALA	C	18	36.883	-17.167	59.956	1.00	39.50	C
ATOM	2624	O	ALA	C	18	36.149	-16.676	59.094	1.00	38.11	O
ATOM	2625	CB	ALA	C	18	35.918	-16.666	62.211	1.00	37.31	C
ATOM	2626	N	SER	C	19	37.537	-18.319	59.802	1.00	42.72	N
ATOM	2627	CA	SER	C	19	37.423	-19.142	58.587	1.00	45.98	C
ATOM	2628	C	SER	C	19	35.949	-19.410	58.282	1.00	46.99	C
ATOM	2629	O	SER	C	19	35.413	-20.463	58.621	1.00	47.77	O
ATOM	2630	CB	SER	C	19	38.179	-20.465	58.762	1.00	46.10	C
ATOM	2631	OG	SER	C	19	38.854	-20.507	60.016	1.00	47.20	O
ATOM	2632	N	GLN	C	20	35.311	-18.429	57.652	1.00	47.66	N
ATOM	2633	CA	GLN	C	20	33.899	-18.460	57.315	1.00	48.47	C
ATOM	2634	C	GLN	C	20	32.951	-18.862	58.434	1.00	49.07	C
ATOM	2635	O	GLN	C	20	31.822	-19.313	58.211	1.00	48.95	O
ATOM	2636	CB	GLN	C	20	33.644	-19.197	56.009	1.00	48.86	C
ATOM	2637	CG	GLN	C	20	33.912	-18.280	54.822	1.00	50.12	C
ATOM	2638	CD	GLN	C	20	33.590	-16.817	55.143	1.00	49.90	C
ATOM	2639	OE1	GLN	C	20	32.512	-16.500	55.653	1.00	48.89	O
ATOM	2640	NE2	GLN	C	20	34.539	-15.929	54.874	1.00	49.91	N
ATOM	2641	N	LYS	C	21	33.394	-18.552	59.646	1.00	49.87	N
ATOM	2642	CA	LYS	C	21	32.643	-18.806	60.865	1.00	49.80	C
ATOM	2643	C	LYS	C	21	32.109	-17.426	61.260	1.00	49.40	C
ATOM	2644	O	LYS	C	21	32.336	-16.440	60.539	1.00	49.21	O
ATOM	2645	CB	LYS	C	21	33.576	-19.353	61.956	1.00	49.61	C
ATOM	2646	CG	LYS	C	21	34.386	-20.576	61.548	1.00	46.89	C
ATOM	2647	CD	LYS	C	21	35.843	-20.444	61.974	1.00	46.08	C
ATOM	2648	CE	LYS	C	21	36.618	-21.710	61.648	1.00	47.91	C
ATOM	2649	NZ	LYS	C	21	38.048	-21.682	62.078	1.00	46.72	N
ATOM	2650	N	LYS	C	22	31.362	-17.356	62.360	1.00	48.20	N
ATOM	2651	CA	LYS	C	22	30.802	-16.088	62.824	1.00	45.14	C
ATOM	2652	C	LYS	C	22	31.290	-15.787	64.231	1.00	43.93	C
ATOM	2653	O	LYS	C	22	32.382	-16.217	64.596	1.00	43.66	O
ATOM	2654	CB	LYS	C	22	29.275	-16.113	62.749	1.00	42.50	C
ATOM	2655	CG	LYS	C	22	28.761	-16.285	61.331	1.00	41.16	C
ATOM	2656	CD	LYS	C	22	29.298	-15.185	60.430	1.00	38.60	C
ATOM	2657	CE	LYS	C	22	29.385	-15.635	58.987	1.00	38.26	C
ATOM	2658	NZ	LYS	C	22	30.447	-16.661	58.796	1.00	37.88	N
ATOM	2659	N	SER	C	23	30.498	-15.058	65.014	1.00	42.70	N
ATOM	2660	CA	SER	C	23	30.877	-14.703	66.379	1.00	42.40	C

FIG. 53-46

ATOM	2662	O	SER	C	23	30.501	-16.619	67.785	1.00	41.43	O
ATOM	2663	CB	SER	C	23	29.721	-14.002	67.094	1.00	43.85	C
ATOM	2664	OG	SER	C	23	30.151	-13.435	68.323	1.00	45.83	O
ATOM	2665	N	ILE	C	24	32.624	-16.170	67.170	1.00	40.65	N
ATOM	2666	CA	ILE	C	24	33.211	-17.292	67.883	1.00	39.11	C
ATOM	2667	C	ILE	C	24	34.438	-16.778	68.623	1.00	37.20	C
ATOM	2668	O	ILE	C	24	34.987	-15.740	68.265	1.00	37.00	O
ATOM	2669	CB	ILE	C	24	33.622	-18.410	66.912	1.00	39.97	C
ATOM	2670	CG1	ILE	C	24	34.679	-17.899	65.928	1.00	39.87	C
ATOM	2671	CG2	ILE	C	24	32.394	-18.933	66.166	1.00	40.37	C
ATOM	2672	CD1	ILE	C	24	35.315	-18.996	65.107	1.00	39.02	C
ATOM	2673	N	GLN	C	25	34.856	-17.496	69.659	1.00	35.82	N
ATOM	2674	CA	GLN	C	25	36.010	-17.093	70.459	1.00	33.47	C
ATOM	2675	C	GLN	C	25	37.230	-16.775	69.597	1.00	30.61	C
ATOM	2676	O	GLN	C	25	37.394	-17.331	68.507	1.00	29.53	O
ATOM	2677	CB	GLN	C	25	36.355	-18.178	71.491	1.00	34.46	C
ATOM	2678	CG	GLN	C	25	36.219	-17.741	72.957	1.00	37.05	C
ATOM	2679	CD	GLN	C	25	34.773	-17.505	73.392	1.00	38.55	C
ATOM	2680	OE1	GLN	C	25	33.988	-16.890	72.673	1.00	38.36	O
ATOM	2681	NE2	GLN	C	25	34.424	-17.986	74.582	1.00	39.56	N
ATOM	2682	N	PHE	C	26	38.043	-15.837	70.075	1.00	27.82	N
ATOM	2683	CA	PHE	C	26	39.261	-15.427	69.387	1.00	25.86	C
ATOM	2684	C	PHE	C	26	40.150	-14.777	70.426	1.00	24.69	C
ATOM	2685	O	PHE	C	26	39.685	-14.460	71.523	1.00	25.10	O
ATOM	2686	CB	PHE	C	26	38.952	-14.401	68.287	1.00	24.48	C
ATOM	2687	CG	PHE	C	26	38.682	-13.009	68.807	1.00	21.65	C
ATOM	2688	CD1	PHE	C	26	37.448	-12.679	69.350	1.00	19.79	C
ATOM	2689	CD2	PHE	C	26	39.675	-12.036	68.768	1.00	19.32	C
ATOM	2690	CE1	PHE	C	26	37.206	-11.406	69.847	1.00	17.63	C
ATOM	2691	CE2	PHE	C	26	39.438	-10.763	69.265	1.00	17.64	C
ATOM	2692	CZ	PHE	C	26	38.204	-10.448	69.806	1.00	16.15	C
ATOM	2693	N	HIS	C	27	41.430	-14.617	70.095	1.00	23.03	N
ATOM	2694	CA	HIS	C	27	42.398	-13.960	70.978	1.00	21.63	C
ATOM	2695	C	HIS	C	27	43.682	-13.568	70.255	1.00	20.47	C
ATOM	2696	O	HIS	C	27	44.269	-14.373	69.526	1.00	19.01	O
ATOM	2697	CB	HIS	C	27	42.706	-14.766	72.257	1.00	22.61	C
ATOM	2698	CG	HIS	C	27	42.699	-16.257	72.074	1.00	26.73	C
ATOM	2699	ND1	HIS	C	27	43.820	-16.973	71.725	1.00	27.44	N
ATOM	2700	CD2	HIS	C	27	41.701	-17.163	72.223	1.00	28.73	C
ATOM	2701	CE1	HIS	C	27	43.516	-18.261	71.666	1.00	28.75	C
ATOM	2702	NE2	HIS	C	27	42.239	-18.400	71.962	1.00	29.75	N
ATOM	2703	N	TRP	C	28	44.048	-12.294	70.396	1.00	19.19	N
ATOM	2704	CA	TRP	C	28	45.249	-11.734	69.793	1.00	18.50	C
ATOM	2705	C	TRP	C	28	46.384	-11.806	70.810	1.00	19.12	C
ATOM	2706	O	TRP	C	28	46.189	-11.505	71.989	1.00	18.57	O
ATOM	2707	CB	TRP	C	28	45.010	-10.277	69.361	1.00	15.67	C
ATOM	2708	CG	TRP	C	28	44.134	-10.125	68.144	1.00	12.38	C
ATOM	2709	CD1	TRP	C	28	42.769	-10.196	68.098	1.00	11.68	C
ATOM	2710	CD2	TRP	C	28	44.569	-9.884	66.796	1.00	11.77	C
ATOM	2711	NE1	TRP	C	28	42.326	-10.016	66.805	1.00	11.45	N
ATOM	2712	CE2	TRP	C	28	43.408	-9.818	65.985	1.00	11.23	C
ATOM	2713	CE3	TRP	C	28	45.823	-9.718	66.185	1.00	12.46	C
ATOM	2714	CZ2	TRP	C	28	43.467	-9.592	64.603	1.00	8.94	C
ATOM	2715	CZ3	TRP	C	28	45.880	-9.497	64.806	1.00	10.11	C
ATOM	2716	CH2	TRP	C	28	44.705	-9.435	64.034	1.00	8.40	C
ATOM	2717	N	LYS	C	29	47.566	-12.190	70.336	1.00	20.29	N
ATOM	2718	CA	LYS	C	29	48.758	-12.338	71.165	1.00	21.63	C
ATOM	2719	C	LYS	C	29	49.976	-11.752	70.449	1.00	22.44	C
ATOM	2720	O	LYS	C	29	49.942	-11.521	69.242	1.00	24.06	O
ATOM	2721	CB	LYS	C	29	49.039	-13.827	71.405	1.00	22.39	C
ATOM	2722	CG	LYS	C	29	48.112	-14.554	72.354	1.00	22.12	C
ATOM	2723	CD	LYS	C	29	48.477	-16.031	72.387	1.00	21.48	C
ATOM	2724	CE	LYS	C	29	47.609	-16.835	73.353	1.00	21.29	C
ATOM	2725	NZ	LYS	C	29	47.777	-18.307	73.142	1.00	20.24	N
ATOM	2726	N	ASN	C	30	51.060	-11.541	71.184	1.00	23.38	N
ATOM	2727	CA	ASN	C	30	52.287	-11.026	70.584	1.00	25.47	C
ATOM	2728	C	ASN	C	30	53.269	-12.185	70.432	1.00	26.26	C
ATOM	2729	O	ASN	C	30	52.995	-13.297	70.889	1.00	25.69	O
ATOM	2730	CB	ASN	C	30	52.890	-9.893	71.419	1.00	27.31	C
ATOM	2731	CG	ASN	C	30	53.683	-10.385	72.611	1.00	30.17	C

FIG. 53-47

ATOM	2733	ND2	ASN	C	30	54.669	-9.604	73.011	1.00	35.07	N
ATOM	2734	N	SER	C	31	54.432	-11.922	69.846	1.00	27.26	N
ATOM	2735	CA	SER	C	31	55.423	-12.973	69.614	1.00	27.23	C
ATOM	2736	C	SER	C	31	55.890	-13.745	70.852	1.00	27.63	C
ATOM	2737	O	SER	C	31	56.648	-14.712	70.731	1.00	28.49	O
ATOM	2738	CB	SER	C	31	56.625	-12.409	68.846	1.00	24.59	C
ATOM	2739	OG	SER	C	31	57.292	-11.412	69.589	1.00	22.89	O
ATOM	2740	N	ASN	C	32	55.424	-13.337	72.030	1.00	27.00	N
ATOM	2741	CA	ASN	C	32	55.819	-13.990	73.282	1.00	25.25	C
ATOM	2742	C	ASN	C	32	54.674	-14.735	73.959	1.00	24.89	C
ATOM	2743	O	ASN	C	32	54.829	-15.233	75.074	1.00	25.83	O
ATOM	2744	CB	ASN	C	32	56.402	-12.962	74.252	1.00	22.99	C
ATOM	2745	CG	ASN	C	32	57.671	-12.330	73.730	1.00	23.34	C
ATOM	2746	OD1	ASN	C	32	58.726	-12.965	73.704	1.00	22.47	O
ATOM	2747	ND2	ASN	C	32	57.577	-11.078	73.293	1.00	23.40	N
ATOM	2748	N	GLN	C	33	53.528	-14.806	73.285	1.00	23.19	N
ATOM	2749	CA	GLN	C	33	52.346	-15.478	73.815	1.00	21.72	C
ATOM	2750	C	GLN	C	33	51.613	-14.691	74.898	1.00	21.12	C
ATOM	2751	O	GLN	C	33	50.781	-15.247	75.623	1.00	21.09	O
ATOM	2752	CB	GLN	C	33	52.696	-16.888	74.306	1.00	21.85	C
ATOM	2753	CG	GLN	C	33	52.808	-17.915	73.190	1.00	20.01	C
ATOM	2754	CD	GLN	C	33	51.465	-18.245	72.588	1.00	18.26	C
ATOM	2755	OE1	GLN	C	33	50.641	-18.909	73.222	1.00	15.86	O
ATOM	2756	NE2	GLN	C	33	51.213	-17.746	71.379	1.00	17.44	N
ATOM	2757	N	ILE	C	34	51.904	-13.397	74.991	1.00	20.10	N
ATOM	2758	CA	ILE	C	34	51.249	-12.535	75.973	1.00	20.03	C
ATOM	2759	C	ILE	C	34	49.875	-12.247	75.382	1.00	19.20	C
ATOM	2760	O	ILE	C	34	49.766	-11.961	74.183	1.00	18.67	O
ATOM	2761	CB	ILE	C	34	51.991	-11.169	76.140	1.00	21.24	C
ATOM	2762	CG1	ILE	C	34	53.457	-11.390	76.543	1.00	21.42	C
ATOM	2763	CG2	ILE	C	34	51.267	-10.287	77.159	1.00	18.98	C
ATOM	2764	CD1	ILE	C	34	53.647	-12.089	77.878	1.00	22.15	C
ATOM	2765	N	LYS	C	35	48.832	-12.372	76.197	1.00	17.71	N
ATOM	2766	CA	LYS	C	35	47.477	-12.111	75.724	1.00	16.90	C
ATOM	2767	C	LYS	C	35	47.226	-10.606	75.642	1.00	17.56	C
ATOM	2768	O	LYS	C	35	47.357	-9.880	76.635	1.00	16.09	O
ATOM	2769	CB	LYS	C	35	46.437	-12.794	76.624	1.00	16.19	C
ATOM	2770	CG	LYS	C	35	46.269	-14.292	76.376	1.00	15.00	C
ATOM	2771	CD	LYS	C	35	46.569	-15.128	77.629	1.00	15.34	C
ATOM	2772	CE	LYS	C	35	45.354	-15.350	78.508	1.00	12.17	C
ATOM	2773	NZ	LYS	C	35	44.915	-14.132	79.227	1.00	16.76	N
ATOM	2774	N	ILE	C	36	46.943	-10.139	74.432	1.00	17.78	N
ATOM	2775	CA	ILE	C	36	46.669	-8.732	74.185	1.00	17.67	C
ATOM	2776	C	ILE	C	36	45.164	-8.505	74.348	1.00	17.41	C
ATOM	2777	O	ILE	C	36	44.725	-7.804	75.263	1.00	18.21	O
ATOM	2778	CB	ILE	C	36	47.058	-8.318	72.729	1.00	17.98	C
ATOM	2779	CG1	ILE	C	36	48.523	-8.684	72.418	1.00	18.20	C
ATOM	2780	CG2	ILE	C	36	46.753	-6.837	72.495	1.00	14.26	C
ATOM	2781	CD1	ILE	C	36	49.593	-7.848	73.124	1.00	12.26	C
ATOM	2782	N	LEU	C	37	44.381	-9.155	73.493	1.00	16.29	N
ATOM	2783	CA	LEU	C	37	42.934	-8.997	73.499	1.00	16.37	C
ATOM	2784	C	LEU	C	37	42.267	-10.310	73.110	1.00	16.74	C
ATOM	2785	O	LEU	C	37	42.914	-11.212	72.584	1.00	19.68	O
ATOM	2786	CB	LEU	C	37	42.552	-7.905	72.486	1.00	16.03	C
ATOM	2787	CG	LEU	C	37	41.095	-7.454	72.339	1.00	15.19	C
ATOM	2788	CD1	LEU	C	37	40.926	-6.062	72.906	1.00	14.65	C
ATOM	2789	CD2	LEU	C	37	40.692	-7.490	70.864	1.00	17.32	C
ATOM	2790	N	GLY	C	38	40.973	-10.416	73.375	1.00	14.89	N
ATOM	2791	CA	GLY	C	38	40.232	-11.611	73.034	1.00	12.10	C
ATOM	2792	C	GLY	C	38	38.857	-11.427	73.608	1.00	11.95	C
ATOM	2793	O	GLY	C	38	38.597	-10.393	74.205	1.00	14.37	O
ATOM	2794	N	ASN	C	39	37.973	-12.401	73.437	1.00	13.54	N
ATOM	2795	CA	ASN	C	39	36.624	-12.295	73.984	1.00	14.16	C
ATOM	2796	C	ASN	C	39	36.331	-13.486	74.885	1.00	14.77	C
ATOM	2797	O	ASN	C	39	37.193	-14.350	75.090	1.00	15.40	O
ATOM	2798	CB	ASN	C	39	35.567	-12.201	72.873	1.00	13.29	C
ATOM	2799	CG	ASN	C	39	35.490	-13.460	72.013	1.00	15.65	C
ATOM	2800	OD1	ASN	C	39	35.976	-14.530	72.397	1.00	15.77	O
ATOM	2801	ND2	ASN	C	39	34.887	-13.333	70.833	1.00	12.54	N
ATOM	2802	N	GLN	C	40	35.120	-13.488	75.459	1.00	13.54	N

FIG. 53-48

ATOM	2804	C	GLN	C	40	33.139	-14.505	76.219	1.00	10.47	C
ATOM	2805	O	GLN	C	40	32.444	-13.954	77.083	1.00	8.94	O
ATOM	2806	CB	GLN	C	40	35.072	-14.327	77.793	1.00	10.26	C
ATOM	2807	CG	GLN	C	40	36.433	-14.944	78.150	1.00	11.63	C
ATOM	2808	CD	GLN	C	40	36.516	-16.464	77.940	1.00	11.02	C
ATOM	2809	OE1	GLN	C	40	37.565	-16.986	77.571	1.00	12.21	O
ATOM	2810	NE2	GLN	C	40	35.424	-17.173	78.204	1.00	7.03	N
ATOM	2811	N	GLY	C	41	32.643	-15.095	75.136	1.00	10.34	N
ATOM	2812	CA	GLY	C	41	31.218	-15.087	74.875	1.00	9.17	C
ATOM	2813	C	GLY	C	41	30.964	-13.757	74.191	1.00	8.46	C
ATOM	2814	O	GLY	C	41	31.518	-13.500	73.129	1.00	9.97	O
ATOM	2815	N	SER	C	42	30.235	-12.872	74.855	1.00	7.34	N
ATOM	2816	CA	SER	C	42	29.917	-11.560	74.310	1.00	5.83	C
ATOM	2817	C	SER	C	42	30.754	-10.420	74.904	1.00	4.58	C
ATOM	2818	O	SER	C	42	30.664	-9.262	74.467	1.00	2.00	O
ATOM	2819	CB	SER	C	42	28.436	-11.281	74.535	1.00	7.62	C
ATOM	2820	OG	SER	C	42	27.652	-12.282	73.918	1.00	7.72	O
ATOM	2821	N	PHE	C	43	31.574	-10.756	75.894	1.00	4.84	N
ATOM	2822	CA	PHE	C	43	32.412	-9.780	76.584	1.00	4.77	C
ATOM	2823	C	PHE	C	43	33.851	-9.771	76.104	1.00	6.41	C
ATOM	2824	O	PHE	C	43	34.401	-10.802	75.740	1.00	8.31	O
ATOM	2825	CB	PHE	C	43	32.394	-10.062	78.085	1.00	3.80	C
ATOM	2826	CG	PHE	C	43	31.019	-10.087	78.668	1.00	2.00	C
ATOM	2827	CD1	PHE	C	43	30.267	-8.927	78.734	1.00	2.00	C
ATOM	2828	CD2	PHE	C	43	30.467	-11.276	79.118	1.00	2.00	C
ATOM	2829	CE1	PHE	C	43	28.986	-8.945	79.232	1.00	2.13	C
ATOM	2830	CE2	PHE	C	43	29.174	-11.313	79.625	1.00	2.00	C
ATOM	2831	CZ	PHE	C	43	28.429	-10.145	79.682	1.00	4.36	C
ATOM	2832	N	LEU	C	44	34.468	-8.598	76.133	1.00	8.65	N
ATOM	2833	CA	LEU	C	44	35.851	-8.448	75.712	1.00	10.75	C
ATOM	2834	C	LEU	C	44	36.755	-8.770	76.898	1.00	10.90	C
ATOM	2835	O	LEU	C	44	36.357	-8.616	78.042	1.00	11.48	O
ATOM	2836	CB	LEU	C	44	36.105	-7.006	75.268	1.00	12.86	C
ATOM	2837	CG	LEU	C	44	37.428	-6.748	74.547	1.00	14.62	C
ATOM	2838	CD1	LEU	C	44	37.262	-7.166	73.088	1.00	15.13	C
ATOM	2839	CD2	LEU	C	44	37.837	-5.277	74.664	1.00	13.01	C
ATOM	2840	N	THR	C	45	37.973	-9.207	76.618	1.00	11.50	N
ATOM	2841	CA	THR	C	45	38.928	-9.525	77.659	1.00	14.24	C
ATOM	2842	C	THR	C	45	40.278	-9.018	77.191	1.00	16.99	C
ATOM	2843	O	THR	C	45	40.656	-9.203	76.017	1.00	16.97	O
ATOM	2844	CB	THR	C	45	39.036	-11.062	77.942	1.00	15.05	C
ATOM	2845	OG1	THR	C	45	39.389	-11.768	76.743	1.00	15.68	O
ATOM	2846	CG2	THR	C	45	37.724	-11.612	78.507	1.00	14.28	C
ATOM	2847	N	LYS	C	46	40.980	-8.336	78.091	1.00	17.91	N
ATOM	2848	CA	LYS	C	46	42.301	-7.808	77.788	1.00	17.33	C
ATOM	2849	C	LYS	C	46	43.265	-8.506	78.714	1.00	17.01	C
ATOM	2850	O	LYS	C	46	42.937	-8.764	79.875	1.00	18.56	O
ATOM	2851	CB	LYS	C	46	42.372	-6.296	78.018	1.00	18.52	C
ATOM	2852	CG	LYS	C	46	41.455	-5.474	77.133	1.00	18.34	C
ATOM	2853	CD	LYS	C	46	41.807	-4.003	77.226	1.00	17.51	C
ATOM	2854	CE	LYS	C	46	40.899	-3.181	76.336	1.00	19.67	C
ATOM	2855	NZ	LYS	C	46	41.328	-1.760	76.203	1.00	18.93	N
ATOM	2856	N	GLY	C	47	44.426	-8.858	78.184	1.00	16.02	N
ATOM	2857	CA	GLY	C	47	45.426	-9.524	78.985	1.00	16.47	C
ATOM	2858	C	GLY	C	47	46.391	-8.515	79.565	1.00	16.67	C
ATOM	2859	O	GLY	C	47	46.124	-7.308	79.534	1.00	16.82	O
ATOM	2860	N	PRO	C	48	47.519	-8.981	80.125	1.00	16.94	N
ATOM	2861	CA	PRO	C	48	48.571	-8.155	80.732	1.00	16.26	C
ATOM	2862	C	PRO	C	48	49.466	-7.404	79.726	1.00	14.98	C
ATOM	2863	O	PRO	C	48	50.529	-6.903	80.094	1.00	15.58	O
ATOM	2864	CB	PRO	C	48	49.398	-9.191	81.509	1.00	14.81	C
ATOM	2865	CG	PRO	C	48	48.439	-10.289	81.772	1.00	14.85	C
ATOM	2866	CD	PRO	C	48	47.736	-10.400	80.455	1.00	15.47	C
ATOM	2867	N	SER	C	49	49.050	-7.304	78.472	1.00	14.68	N
ATOM	2868	CA	SER	C	49	49.878	-6.634	77.473	1.00	16.42	C
ATOM	2869	C	SER	C	49	50.152	-5.176	77.805	1.00	17.17	C
ATOM	2870	O	SER	C	49	49.384	-4.538	78.532	1.00	17.47	O
ATOM	2871	CB	SER	C	49	49.221	-6.685	76.102	1.00	17.09	C
ATOM	2872	OG	SER	C	49	48.311	-5.609	75.922	1.00	16.81	O

FIG. 53-49

ATOM	2875	C	LYS	C	50	50.643	-2.354	76.543	1.00	18.94	C
ATOM	2876	O	LYS	C	50	50.795	-1.138	76.500	1.00	20.82	O
ATOM	2877	CB	LYS	C	50	53.026	-2.991	77.078	1.00	21.26	C
ATOM	2878	CG	LYS	C	50	53.540	-1.632	77.536	1.00	24.37	C
ATOM	2879	CD	LYS	C	50	55.018	-1.463	77.232	1.00	27.45	C
ATOM	2880	CE	LYS	C	50	55.500	-0.048	77.536	1.00	28.49	C
ATOM	2881	NZ	LYS	C	50	56.905	0.162	77.095	1.00	25.44	N
ATOM	2882	N	LEU	C	51	49.707	-2.986	75.837	1.00	19.14	N
ATOM	2883	CA	LEU	C	51	48.735	-2.298	74.985	1.00	16.80	C
ATOM	2884	C	LEU	C	51	47.399	-2.255	75.700	1.00	18.11	C
ATOM	2885	O	LEU	C	51	46.454	-1.654	75.203	1.00	18.22	O
ATOM	2886	CB	LEU	C	51	48.516	-3.065	73.676	1.00	12.49	C
ATOM	2887	CG	LEU	C	51	49.483	-2.941	72.498	1.00	11.96	C
ATOM	2888	CD1	LEU	C	51	50.928	-3.201	72.901	1.00	9.37	C
ATOM	2889	CD2	LEU	C	51	49.034	-3.900	71.410	1.00	8.92	C
ATOM	2890	N	ASN	C	52	47.318	-2.910	76.856	1.00	19.44	N
ATOM	2891	CA	ASN	C	52	46.075	-3.000	77.623	1.00	21.42	C
ATOM	2892	C	ASN	C	52	45.154	-1.793	77.526	1.00	21.58	C
ATOM	2893	O	ASN	C	52	43.969	-1.910	77.186	1.00	21.08	O
ATOM	2894	CB	ASN	C	52	46.374	-3.286	79.092	1.00	22.65	C
ATOM	2895	CG	ASN	C	52	45.115	-3.524	79.897	1.00	25.24	C
ATOM	2896	OD1	ASN	C	52	44.399	-2.586	80.245	1.00	26.00	O
ATOM	2897	ND2	ASN	C	52	44.819	-4.787	80.169	1.00	27.41	N
ATOM	2898	N	ASP	C	53	45.724	-0.635	77.821	1.00	22.99	N
ATOM	2899	CA	ASP	C	53	45.017	0.641	77.810	1.00	22.76	C
ATOM	2900	C	ASP	C	53	44.612	1.142	76.424	1.00	20.28	C
ATOM	2901	O	ASP	C	53	43.583	1.808	76.287	1.00	20.58	O
ATOM	2902	CB	ASP	C	53	45.883	1.688	78.510	1.00	27.19	C
ATOM	2903	CG	ASP	C	53	47.369	1.438	78.304	1.00	32.20	C
ATOM	2904	OD1	ASP	C	53	47.834	1.474	77.140	1.00	34.77	O
ATOM	2905	OD2	ASP	C	53	48.063	1.153	79.304	1.00	33.85	O
ATOM	2906	N	ARG	C	54	45.387	0.776	75.404	1.00	16.44	N
ATOM	2907	CA	ARG	C	54	45.138	1.214	74.035	1.00	14.46	C
ATOM	2908	C	ARG	C	54	44.498	0.223	73.052	1.00	15.26	C
ATOM	2909	O	ARG	C	54	43.934	0.631	72.024	1.00	14.48	O
ATOM	2910	CB	ARG	C	54	46.438	1.769	73.453	1.00	13.85	C
ATOM	2911	CG	ARG	C	54	46.969	2.981	74.207	1.00	10.39	C
ATOM	2912	CD	ARG	C	54	48.348	3.384	73.736	1.00	9.86	C
ATOM	2913	NE	ARG	C	54	49.387	2.400	74.043	1.00	10.92	N
ATOM	2914	CZ	ARG	C	54	49.902	1.546	73.159	1.00	11.74	C
ATOM	2915	NH1	ARG	C	54	49.465	1.539	71.903	1.00	10.30	N
ATOM	2916	NH2	ARG	C	54	50.884	0.731	73.521	1.00	11.51	N
ATOM	2917	N	ALA	C	55	44.571	-1.066	73.362	1.00	15.91	N
ATOM	2918	CA	ALA	C	55	44.012	-2.105	72.505	1.00	15.65	C
ATOM	2919	C	ALA	C	55	42.538	-2.289	72.806	1.00	16.53	C
ATOM	2920	O	ALA	C	55	42.146	-2.312	73.971	1.00	16.52	O
ATOM	2921	CB	ALA	C	55	44.743	-3.414	72.735	1.00	16.20	C
ATOM	2922	N	ASP	C	56	41.731	-2.424	71.759	1.00	16.49	N
ATOM	2923	CA	ASP	C	56	40.289	-2.635	71.893	1.00	15.07	C
ATOM	2924	C	ASP	C	56	39.804	-3.354	70.648	1.00	13.98	C
ATOM	2925	O	ASP	C	56	40.599	-3.615	69.741	1.00	13.65	O
ATOM	2926	CB	ASP	C	56	39.550	-1.316	72.086	1.00	15.99	C
ATOM	2927	CG	ASP	C	56	38.751	-1.297	73.365	1.00	19.33	C
ATOM	2928	OD1	ASP	C	56	37.587	-1.749	73.338	1.00	18.87	O
ATOM	2929	OD2	ASP	C	56	39.301	-0.865	74.408	1.00	22.07	O
ATOM	2930	N	SER	C	57	38.512	-3.642	70.568	1.00	13.07	N
ATOM	2931	CA	SER	C	57	37.991	-4.388	69.421	1.00	12.85	C
ATOM	2932	C	SER	C	57	36.819	-3.677	68.735	1.00	12.16	C
ATOM	2933	O	SER	C	57	36.633	-2.468	68.873	1.00	9.84	O
ATOM	2934	CB	SER	C	57	37.558	-5.783	69.913	1.00	12.60	C
ATOM	2935	OG	SER	C	57	37.440	-6.721	68.858	1.00	14.97	O
ATOM	2936	N	ARG	C	58	36.075	-4.420	67.925	1.00	12.21	N
ATOM	2937	CA	ARG	C	58	34.897	-3.870	67.286	1.00	12.94	C
ATOM	2938	C	ARG	C	58	33.805	-4.937	67.358	1.00	12.65	C
ATOM	2939	O	ARG	C	58	33.483	-5.602	66.386	1.00	12.66	O
ATOM	2940	CB	ARG	C	58	35.180	-3.396	65.860	1.00	13.06	C
ATOM	2941	CG	ARG	C	58	34.391	-2.125	65.519	1.00	15.59	C
ATOM	2942	CD	ARG	C	58	34.999	-1.326	64.364	1.00	16.20	C
ATOM	2943	NE	ARG	C	58	34.536	0.057	64.369	1.00	16.31	N
ATOM	2944	CZ	ARG	C	58	34.975	0.983	65.220	1.00	19.59	C

FIG. 53-50

ATOM	2946	NH2	ARG	C	58	34.474	2.211	65.191	1.00	21.55	N
ATOM	2947	N	ARG	C	59	33.238	-5.063	68.551	1.00	13.04	N
ATOM	2948	CA	ARG	C	59	32.187	-6.030	68.879	1.00	13.46	C
ATOM	2949	C	ARG	C	59	31.102	-6.069	67.820	1.00	13.81	C
ATOM	2950	O	ARG	C	59	30.430	-7.077	67.640	1.00	12.88	O
ATOM	2951	CB	ARG	C	59	31.559	-5.658	70.225	1.00	12.47	C
ATOM	2952	CG	ARG	C	59	32.574	-5.123	71.230	1.00	16.63	C
ATOM	2953	CD	ARG	C	59	31.925	-4.363	72.377	1.00	15.86	C
ATOM	2954	NE	ARG	C	59	31.447	-5.274	73.399	1.00	14.58	N
ATOM	2955	CZ	ARG	C	59	32.094	-5.521	74.530	1.00	15.29	C
ATOM	2956	NH1	ARG	C	59	33.242	-4.907	74.793	1.00	11.07	N
ATOM	2957	NH2	ARG	C	59	31.651	-6.473	75.336	1.00	16.27	N
ATOM	2958	N	SER	C	60	30.955	-4.952	67.119	1.00	15.22	N
ATOM	2959	CA	SER	C	60	29.957	-4.780	66.074	1.00	14.35	C
ATOM	2960	C	SER	C	60	30.115	-5.787	64.956	1.00	14.12	C
ATOM	2961	O	SER	C	60	29.126	-6.249	64.391	1.00	14.24	O
ATOM	2962	CB	SER	C	60	30.079	-3.373	65.491	1.00	13.29	C
ATOM	2963	OG	SER	C	60	30.297	-2.413	66.513	1.00	12.44	O
ATOM	2964	N	LEU	C	61	31.365	-6.114	64.643	1.00	13.35	N
ATOM	2965	CA	LEU	C	61	31.698	-7.036	63.562	1.00	12.58	C
ATOM	2966	C	LEU	C	61	31.890	-8.488	63.994	1.00	12.89	C
ATOM	2967	O	LEU	C	61	32.214	-9.344	63.171	1.00	11.27	O
ATOM	2968	CB	LEU	C	61	32.970	-6.542	62.861	1.00	12.99	C
ATOM	2969	CG	LEU	C	61	32.986	-5.102	62.316	1.00	12.37	C
ATOM	2970	CD1	LEU	C	61	34.367	-4.729	61.845	1.00	10.21	C
ATOM	2971	CD2	LEU	C	61	32.002	-4.958	61.179	1.00	13.32	C
ATOM	2972	N	TRP	C	62	31.653	-8.782	65.267	1.00	15.00	N
ATOM	2973	CA	TRP	C	62	31.844	-10.137	65.768	1.00	15.79	C
ATOM	2974	C	TRP	C	62	30.877	-11.111	65.138	1.00	17.16	C
ATOM	2975	O	TRP	C	62	31.280	-12.199	64.708	1.00	16.99	O
ATOM	2976	CB	TRP	C	62	31.737	-10.182	67.289	1.00	14.89	C
ATOM	2977	CG	TRP	C	62	32.910	-9.553	67.997	1.00	12.85	C
ATOM	2978	CD1	TRP	C	62	33.989	-8.952	67.423	1.00	10.02	C
ATOM	2979	CD2	TRP	C	62	33.113	-9.470	69.418	1.00	11.04	C
ATOM	2980	NE1	TRP	C	62	34.846	-8.498	68.392	1.00	9.91	N
ATOM	2981	CE2	TRP	C	62	34.331	-8.798	69.625	1.00	8.87	C
ATOM	2982	CE3	TRP	C	62	32.379	-9.899	70.531	1.00	10.38	C
ATOM	2983	CZ2	TRP	C	62	34.840	-8.541	70.902	1.00	9.83	C
ATOM	2984	CZ3	TRP	C	62	32.884	-9.648	71.801	1.00	11.71	C
ATOM	2985	CH2	TRP	C	62	34.104	-8.971	71.975	1.00	10.91	C
ATOM	2986	N	ASP	C	63	29.619	-10.689	65.023	1.00	18.68	N
ATOM	2987	CA	ASP	C	63	28.560	-11.504	64.424	1.00	19.37	C
ATOM	2988	C	ASP	C	63	28.674	-11.662	62.905	1.00	19.18	C
ATOM	2989	O	ASP	C	63	27.858	-12.339	62.270	1.00	18.52	O
ATOM	2990	CB	ASP	C	63	27.200	-10.939	64.801	1.00	20.43	C
ATOM	2991	CG	ASP	C	63	27.000	-10.882	66.293	1.00	22.49	C
ATOM	2992	OD1	ASP	C	63	27.551	-11.753	67.000	1.00	22.01	O
ATOM	2993	OD2	ASP	C	63	26.310	-9.950	66.760	1.00	23.27	O
ATOM	2994	N	GLN	C	64	29.665	-10.993	62.324	1.00	20.21	N
ATOM	2995	CA	GLN	C	64	29.946	-11.072	60.894	1.00	21.25	C
ATOM	2996	C	GLN	C	64	31.237	-11.861	60.695	1.00	21.70	C
ATOM	2997	O	GLN	C	64	31.689	-12.079	59.566	1.00	21.95	O
ATOM	2998	CB	GLN	C	64	30.060	-9.680	60.282	1.00	22.27	C
ATOM	2999	CG	GLN	C	64	28.713	-9.092	59.868	1.00	27.63	C
ATOM	3000	CD	GLN	C	64	27.617	-9.343	60.897	1.00	31.22	C
ATOM	3001	OE1	GLN	C	64	27.598	-8.736	61.971	1.00	32.64	O
ATOM	3002	NE2	GLN	C	64	26.718	-10.265	60.585	1.00	34.04	N
ATOM	3003	N	GLY	C	65	31.812	-12.304	61.813	1.00	21.06	N
ATOM	3004	CA	GLY	C	65	33.024	-13.090	61.776	1.00	19.23	C
ATOM	3005	C	GLY	C	65	34.316	-12.317	61.841	1.00	19.06	C
ATOM	3006	O	GLY	C	65	35.374	-12.928	61.888	1.00	20.04	O
ATOM	3007	N	ASN	C	66	34.260	-10.991	61.859	1.00	18.88	N
ATOM	3008	CA	ASN	C	66	35.487	-10.211	61.918	1.00	19.26	C
ATOM	3009	C	ASN	C	66	35.736	-9.585	63.298	1.00	18.39	C
ATOM	3010	O	ASN	C	66	34.952	-8.759	63.775	1.00	17.22	O
ATOM	3011	CB	ASN	C	66	35.504	-9.142	60.816	1.00	22.32	C
ATOM	3012	CG	ASN	C	66	36.770	-8.278	60.848	1.00	25.70	C
ATOM	3013	OD1	ASN	C	66	37.901	-8.784	60.827	1.00	26.05	O
ATOM	3014	ND2	ASN	C	66	36.578	-6.968	60.900	1.00	26.51	N
ATOM	3015	N	PHE	C	67	36.837	-9.996	63.930	1.00	17.78	N

FIG. 53-51

ATOM	3017	C	PHE	C	67	38.629	-8.895	65.173	1.00	15.42	C
ATOM	3018	O	PHE	C	67	39.629	-9.578	65.392	1.00	14.55	O
ATOM	3019	CB	PHE	C	67	37.261	-10.635	66.284	1.00	15.35	C
ATOM	3020	CG	PHE	C	67	36.638	-11.919	65.821	1.00	14.85	C
ATOM	3021	CD1	PHE	C	67	37.409	-12.884	65.171	1.00	15.03	C
ATOM	3022	CD2	PHE	C	67	35.299	-12.180	66.063	1.00	14.06	C
ATOM	3023	CE1	PHE	C	67	36.866	-14.085	64.773	1.00	13.69	C
ATOM	3024	CE2	PHE	C	67	34.737	-13.386	65.668	1.00	15.16	C
ATOM	3025	CZ	PHE	C	67	35.527	-14.343	65.021	1.00	15.92	C
ATOM	3026	N	PRO	C	68	38.709	-7.580	64.908	1.00	14.57	N
ATOM	3027	CA	PRO	C	68	39.975	-6.859	64.797	1.00	12.80	C
ATOM	3028	C	PRO	C	68	40.599	-6.423	66.117	1.00	11.73	C
ATOM	3029	O	PRO	C	68	39.979	-6.528	67.182	1.00	10.66	O
ATOM	3030	CB	PRO	C	68	39.581	-5.649	63.959	1.00	11.75	C
ATOM	3031	CG	PRO	C	68	38.226	-5.342	64.481	1.00	10.44	C
ATOM	3032	CD	PRO	C	68	37.576	-6.702	64.552	1.00	12.41	C
ATOM	3033	N	LEU	C	69	41.823	-5.905	66.012	1.00	10.60	N
ATOM	3034	CA	LEU	C	69	42.595	-5.395	67.140	1.00	10.14	C
ATOM	3035	C	LEU	C	69	42.793	-3.921	66.813	1.00	12.09	C
ATOM	3036	O	LEU	C	69	43.527	-3.583	65.870	1.00	14.51	O
ATOM	3037	CB	LEU	C	69	43.977	-6.051	67.181	1.00	7.25	C
ATOM	3038	CG	LEU	C	69	44.752	-6.202	68.495	1.00	6.79	C
ATOM	3039	CD1	LEU	C	69	46.237	-6.243	68.179	1.00	5.65	C
ATOM	3040	CD2	LEU	C	69	44.449	-5.091	69.477	1.00	2.33	C
ATOM	3041	N	ILE	C	70	42.145	-3.038	67.558	1.00	11.69	N
ATOM	3042	CA	ILE	C	70	42.286	-1.613	67.293	1.00	11.41	C
ATOM	3043	C	ILE	C	70	43.276	-0.974	68.255	1.00	11.83	C
ATOM	3044	O	ILE	C	70	42.932	-0.657	69.399	1.00	13.17	O
ATOM	3045	CB	ILE	C	70	40.937	-0.893	67.367	1.00	10.01	C
ATOM	3046	CG1	ILE	C	70	40.002	-1.450	66.297	1.00	5.60	C
ATOM	3047	CG2	ILE	C	70	41.129	0.603	67.162	1.00	11.59	C
ATOM	3048	CD1	ILE	C	70	38.668	-0.798	66.297	1.00	5.00	C
ATOM	3049	N	ILE	C	71	44.502	-0.778	67.784	1.00	11.80	N
ATOM	3050	CA	ILE	C	71	45.554	-0.186	68.606	1.00	11.31	C
ATOM	3051	C	ILE	C	71	45.654	1.335	68.491	1.00	12.62	C
ATOM	3052	O	ILE	C	71	46.256	1.864	67.552	1.00	12.80	O
ATOM	3053	CB	ILE	C	71	46.927	-0.782	68.265	1.00	8.18	C
ATOM	3054	CG1	ILE	C	71	46.898	-2.302	68.407	1.00	3.27	C
ATOM	3055	CG2	ILE	C	71	47.993	-0.178	69.173	1.00	7.17	C
ATOM	3056	CD1	ILE	C	71	48.127	-2.966	67.867	1.00	3.36	C
ATOM	3057	N	LYS	C	72	45.067	2.046	69.447	1.00	13.66	N
ATOM	3058	CA	LYS	C	72	45.149	3.493	69.412	1.00	13.73	C
ATOM	3059	C	LYS	C	72	46.495	3.954	69.953	1.00	12.76	C
ATOM	3060	O	LYS	C	72	47.207	3.195	70.607	1.00	11.55	O
ATOM	3061	CB	LYS	C	72	43.982	4.141	70.152	1.00	15.88	C
ATOM	3062	CG	LYS	C	72	43.750	3.668	71.563	1.00	18.88	C
ATOM	3063	CD	LYS	C	72	42.410	4.193	72.055	1.00	20.34	C
ATOM	3064	CE	LYS	C	72	41.521	3.058	72.523	1.00	23.79	C
ATOM	3065	NZ	LYS	C	72	41.542	1.869	71.616	1.00	26.10	N
ATOM	3066	N	ASN	C	73	46.870	5.173	69.592	1.00	13.66	N
ATOM	3067	CA	ASN	C	73	48.131	5.774	70.005	1.00	15.48	C
ATOM	3068	C	ASN	C	73	49.329	4.844	69.869	1.00	14.73	C
ATOM	3069	O	ASN	C	73	49.939	4.445	70.860	1.00	14.86	O
ATOM	3070	CB	ASN	C	73	48.036	6.315	71.430	1.00	16.97	C
ATOM	3071	CG	ASN	C	73	49.323	6.973	71.893	1.00	20.51	C
ATOM	3072	OD1	ASN	C	73	49.654	6.944	73.088	1.00	23.06	O
ATOM	3073	ND2	ASN	C	73	50.065	7.561	70.955	1.00	19.37	N
ATOM	3074	N	LEU	C	74	49.643	4.469	68.635	1.00	15.11	N
ATOM	3075	CA	LEU	C	74	50.787	3.603	68.388	1.00	14.53	C
ATOM	3076	C	LEU	C	74	52.020	4.234	69.004	1.00	15.55	C
ATOM	3077	O	LEU	C	74	52.154	5.467	69.054	1.00	15.44	O
ATOM	3078	CB	LEU	C	74	51.042	3.419	66.888	1.00	15.89	C
ATOM	3079	CG	LEU	C	74	50.184	2.525	65.982	1.00	15.23	C
ATOM	3080	CD1	LEU	C	74	49.899	1.231	66.696	1.00	16.69	C
ATOM	3081	CD2	LEU	C	74	48.907	3.206	65.600	1.00	14.58	C
ATOM	3082	N	LYS	C	75	52.895	3.388	69.515	1.00	17.06	N
ATOM	3083	CA	LYS	C	75	54.141	3.837	70.105	1.00	19.14	C
ATOM	3084	C	LYS	C	75	55.172	3.037	69.351	1.00	21.30	C
ATOM	3085	O	LYS	C	75	54.886	1.939	68.899	1.00	22.05	O
ATOM	3086	CB	LYS	C	75	54.194	3.493	71.591	1.00	18.92	C

FIG. 53-52

ATOM	3088	CD	LYS	C	75	53.251	3.834	73.890	1.00	16.94	C
ATOM	3089	CE	LYS	C	75	52.035	4.287	74.678	1.00	16.82	C
ATOM	3090	NZ	LYS	C	75	51.586	5.625	74.222	1.00	17.55	N
ATOM	3091	N	ILE	C	76	56.366	3.582	69.179	1.00	23.77	N
ATOM	3092	CA	ILE	C	76	57.397	2.858	68.454	1.00	25.15	C
ATOM	3093	C	ILE	C	76	57.621	1.490	69.093	1.00	25.32	C
ATOM	3094	O	ILE	C	76	57.976	0.527	68.415	1.00	24.60	O
ATOM	3095	CB	ILE	C	76	58.707	3.680	68.393	1.00	26.22	C
ATOM	3096	CG1	ILE	C	76	58.587	4.749	67.303	1.00	27.32	C
ATOM	3097	CG2	ILE	C	76	59.913	2.781	68.102	1.00	25.80	C
ATOM	3098	CD1	ILE	C	76	57.491	5.768	67.529	1.00	26.34	C
ATOM	3099	N	GLU	C	77	57.312	1.403	70.384	1.00	26.79	N
ATOM	3100	CA	GLU	C	77	57.470	0.177	71.167	1.00	27.63	C
ATOM	3101	C	GLU	C	77	56.359	-0.863	70.974	1.00	26.10	C
ATOM	3102	O	GLU	C	77	56.429	-1.959	71.516	1.00	25.20	O
ATOM	3103	CB	GLU	C	77	57.655	0.523	72.655	1.00	29.66	C
ATOM	3104	CG	GLU	C	77	56.645	1.522	73.224	1.00	33.53	C
ATOM	3105	CD	GLU	C	77	56.970	1.950	74.645	1.00	36.75	C
ATOM	3106	OE1	GLU	C	77	57.926	1.408	75.231	1.00	39.53	O
ATOM	3107	OE2	GLU	C	77	56.266	2.820	75.199	1.00	39.29	O
ATOM	3108	N	ASP	C	78	55.346	-0.514	70.192	1.00	25.10	N
ATOM	3109	CA	ASP	C	78	54.249	-1.425	69.893	1.00	23.24	C
ATOM	3110	C	ASP	C	78	54.646	-2.320	68.724	1.00	22.69	C
ATOM	3111	O	ASP	C	78	53.898	-3.220	68.345	1.00	23.77	O
ATOM	3112	CB	ASP	C	78	52.982	-0.659	69.503	1.00	22.41	C
ATOM	3113	CG	ASP	C	78	52.318	0.027	70.677	1.00	22.01	C
ATOM	3114	OD1	ASP	C	78	52.715	-0.188	71.843	1.00	21.08	O
ATOM	3115	OD2	ASP	C	78	51.373	0.797	70.428	1.00	21.00	O
ATOM	3116	N	SER	C	79	55.792	-2.038	68.113	1.00	21.33	N
ATOM	3117	CA	SER	C	79	56.263	-2.832	66.990	1.00	19.92	C
ATOM	3118	C	SER	C	79	56.511	-4.258	67.461	1.00	20.47	C
ATOM	3119	O	SER	C	79	57.421	-4.516	68.258	1.00	19.43	O
ATOM	3120	CB	SER	C	79	57.542	-2.234	66.408	1.00	19.60	C
ATOM	3121	OG	SER	C	79	57.325	-0.905	65.968	1.00	17.97	O
ATOM	3122	N	ASP	C	80	55.683	-5.175	66.972	1.00	20.66	N
ATOM	3123	CA	ASP	C	80	55.773	-6.582	67.333	1.00	21.15	C
ATOM	3124	C	ASP	C	80	55.052	-7.351	66.237	1.00	21.82	C
ATOM	3125	O	ASP	C	80	54.693	-6.772	65.204	1.00	21.49	O
ATOM	3126	CB	ASP	C	80	55.076	-6.815	68.681	1.00	21.40	C
ATOM	3127	CG	ASP	C	80	55.637	-8.016	69.450	1.00	21.01	C
ATOM	3128	OD1	ASP	C	80	56.278	-8.896	68.832	1.00	20.07	O
ATOM	3129	OD2	ASP	C	80	55.421	-8.081	70.685	1.00	18.09	O
ATOM	3130	N	THR	C	81	54.842	-8.645	66.459	1.00	22.92	N
ATOM	3131	CA	THR	C	81	54.162	-9.517	65.506	1.00	22.30	C
ATOM	3132	C	THR	C	81	52.903	-10.027	66.196	1.00	20.64	C
ATOM	3133	O	THR	C	81	52.963	-10.666	67.247	1.00	20.88	O
ATOM	3134	CB	THR	C	81	55.069	-10.684	65.103	1.00	23.98	C
ATOM	3135	OG1	THR	C	81	56.333	-10.165	64.664	1.00	28.26	O
ATOM	3136	CG2	THR	C	81	54.454	-11.474	63.972	1.00	24.03	C
ATOM	3137	N	TYR	C	82	51.757	-9.696	65.624	1.00	19.53	N
ATOM	3138	CA	TYR	C	82	50.485	-10.074	66.205	1.00	18.75	C
ATOM	3139	C	TYR	C	82	49.865	-11.301	65.570	1.00	18.24	C
ATOM	3140	O	TYR	C	82	49.860	-11.462	64.349	1.00	17.98	O
ATOM	3141	CB	TYR	C	82	49.538	-8.865	66.200	1.00	18.14	C
ATOM	3142	CG	TYR	C	82	50.093	-7.730	67.034	1.00	13.90	C
ATOM	3143	CD1	TYR	C	82	49.875	-7.691	68.402	1.00	12.30	C
ATOM	3144	CD2	TYR	C	82	50.951	-6.772	66.473	1.00	14.05	C
ATOM	3145	CE1	TYR	C	82	50.500	-6.746	69.203	1.00	14.07	C
ATOM	3146	CE2	TYR	C	82	51.588	-5.819	67.270	1.00	12.70	C
ATOM	3147	CZ	TYR	C	82	51.360	-5.816	68.640	1.00	13.93	C
ATOM	3148	OH	TYR	C	82	52.008	-4.928	69.472	1.00	13.27	O
ATOM	3149	N	ILE	C	83	49.373	-12.180	66.434	1.00	17.52	N
ATOM	3150	CA	ILE	C	83	48.770	-13.437	66.030	1.00	16.78	C
ATOM	3151	C	ILE	C	83	47.307	-13.513	66.455	1.00	17.28	C
ATOM	3152	O	ILE	C	83	46.974	-13.255	67.610	1.00	17.58	O
ATOM	3153	CB	ILE	C	83	49.540	-14.626	66.652	1.00	15.69	C
ATOM	3154	CG1	ILE	C	83	50.902	-14.800	65.970	1.00	15.70	C
ATOM	3155	CG2	ILE	C	83	48.730	-15.889	66.557	1.00	15.51	C
ATOM	3156	CD1	ILE	C	83	52.029	-13.997	66.604	1.00	11.73	C
ATOM	3157	N	CYS	C	84	46.441	-13.880	65.522	1.00	18.23	N

FIG. 53-53

ATOM	3159	C	CYS	C	84	44.640	-15.483	65.814	1.00	24.15	C
ATOM	3160	O	CYS	C	84	44.618	-16.154	64.766	1.00	22.78	O
ATOM	3161	CB	CYS	C	84	44.188	-13.250	64.777	1.00	21.83	C
ATOM	3162	SG	CYS	C	84	42.428	-13.182	65.225	1.00	25.21	S
ATOM	3163	N	GLU	C	85	44.392	-15.994	67.018	1.00	27.19	N
ATOM	3164	CA	GLU	C	85	44.015	-17.386	67.208	1.00	29.12	C
ATOM	3165	C	GLU	C	85	42.507	-17.549	67.265	1.00	30.85	C
ATOM	3166	O	GLU	C	85	41.885	-17.391	68.319	1.00	29.71	O
ATOM	3167	CB	GLU	C	85	44.665	-17.947	68.475	1.00	28.74	C
ATOM	3168	CG	GLU	C	85	46.187	-17.957	68.433	1.00	31.76	C
ATOM	3169	CD	GLU	C	85	46.835	-18.225	69.780	1.00	34.21	C
ATOM	3170	OE1	GLU	C	85	46.225	-17.912	70.825	1.00	33.71	O
ATOM	3171	OE2	GLU	C	85	47.977	-18.739	69.797	1.00	37.16	O
ATOM	3172	N	VAL	C	86	41.913	-17.733	66.092	1.00	34.16	N
ATOM	3173	CA	VAL	C	86	40.480	-17.974	65.992	1.00	37.67	C
ATOM	3174	C	VAL	C	86	40.445	-19.485	66.212	1.00	40.96	C
ATOM	3175	O	VAL	C	86	41.444	-20.044	66.684	1.00	44.87	O
ATOM	3176	CB	VAL	C	86	39.958	-17.638	64.591	1.00	37.29	C
ATOM	3177	CG1	VAL	C	86	38.469	-17.369	64.643	1.00	38.34	C
ATOM	3178	CG2	VAL	C	86	40.679	-16.434	64.040	1.00	36.92	C
ATOM	3179	N	GLU	C	87	39.352	-20.172	65.894	1.00	41.57	N
ATOM	3180	CA	GLU	C	87	39.351	-21.620	66.098	1.00	41.58	C
ATOM	3181	C	GLU	C	87	40.342	-22.283	65.141	1.00	40.88	C
ATOM	3182	O	GLU	C	87	40.013	-22.639	64.015	1.00	39.29	O
ATOM	3183	CB	GLU	C	87	37.940	-22.198	65.976	1.00	43.78	C
ATOM	3184	CG	GLU	C	87	37.021	-21.792	67.137	1.00	44.89	C
ATOM	3185	CD	GLU	C	87	37.578	-22.178	68.514	1.00	45.97	C
ATOM	3186	OE1	GLU	C	87	37.589	-23.384	68.848	1.00	46.01	O
ATOM	3187	OE2	GLU	C	87	37.994	-21.271	69.269	1.00	45.49	O
ATOM	3188	N	ASP	C	88	41.589	-22.311	65.593	1.00	42.51	N
ATOM	3189	CA	ASP	C	88	42.743	-22.865	64.891	1.00	45.29	C
ATOM	3190	C	ASP	C	88	43.083	-22.359	63.484	1.00	45.77	C
ATOM	3191	O	ASP	C	88	42.784	-23.007	62.477	1.00	47.06	O
ATOM	3192	CB	ASP	C	88	42.730	-24.395	64.926	1.00	47.66	C
ATOM	3193	CG	ASP	C	88	44.050	-24.998	64.468	1.00	50.96	C
ATOM	3194	OD1	ASP	C	88	45.112	-24.378	64.707	1.00	52.73	O
ATOM	3195	OD2	ASP	C	88	44.020	-26.091	63.868	1.00	54.34	O
ATOM	3196	N	GLN	C	89	43.686	-21.173	63.441	1.00	44.42	N
ATOM	3197	CA	GLN	C	89	44.153	-20.531	62.213	1.00	43.08	C
ATOM	3198	C	GLN	C	89	44.946	-19.302	62.657	1.00	42.12	C
ATOM	3199	O	GLN	C	89	44.412	-18.209	62.856	1.00	43.48	O
ATOM	3200	CB	GLN	C	89	43.019	-20.187	61.225	1.00	43.22	C
ATOM	3201	CG	GLN	C	89	42.043	-19.084	61.612	1.00	45.08	C
ATOM	3202	CD	GLN	C	89	41.334	-18.501	60.397	1.00	45.85	C
ATOM	3203	OE1	GLN	C	89	41.128	-19.189	59.398	1.00	48.18	O
ATOM	3204	NE2	GLN	C	89	40.962	-17.236	60.474	1.00	46.49	N
ATOM	3205	N	LYS	C	90	46.231	-19.533	62.887	1.00	39.71	N
ATOM	3206	CA	LYS	C	90	47.156	-18.513	63.353	1.00	36.88	C
ATOM	3207	C	LYS	C	90	47.452	-17.390	62.340	1.00	36.11	C
ATOM	3208	O	LYS	C	90	48.566	-17.305	61.814	1.00	36.72	O
ATOM	3209	CB	LYS	C	90	48.459	-19.207	63.771	1.00	35.10	C
ATOM	3210	CG	LYS	C	90	49.071	-18.718	65.069	1.00	33.77	C
ATOM	3211	CD	LYS	C	90	48.474	-19.386	66.306	1.00	30.81	C
ATOM	3212	CE	LYS	C	90	48.957	-20.826	66.463	1.00	28.79	C
ATOM	3213	NZ	LYS	C	90	48.637	-21.374	67.809	1.00	25.63	N
ATOM	3214	N	GLU	C	91	46.466	-16.542	62.050	1.00	34.49	N
ATOM	3215	CA	GLU	C	91	46.675	-15.426	61.121	1.00	33.21	C
ATOM	3216	C	GLU	C	91	47.696	-14.502	61.797	1.00	32.27	C
ATOM	3217	O	GLU	C	91	47.449	-13.992	62.888	1.00	31.93	O
ATOM	3218	CB	GLU	C	91	45.376	-14.653	60.895	1.00	34.08	C
ATOM	3219	CG	GLU	C	91	44.211	-15.444	60.320	1.00	34.71	C
ATOM	3220	CD	GLU	C	91	42.866	-14.887	60.777	1.00	35.45	C
ATOM	3221	OE1	GLU	C	91	42.403	-15.312	61.851	1.00	37.00	O
ATOM	3222	OE2	GLU	C	91	42.279	-14.020	60.090	1.00	34.33	O
ATOM	3223	N	GLU	C	92	48.831	-14.284	61.149	1.00	30.93	N
ATOM	3224	CA	GLU	C	92	49.898	-13.460	61.715	1.00	29.07	C
ATOM	3225	C	GLU	C	92	50.055	-12.093	61.028	1.00	27.44	C
ATOM	3226	O	GLU	C	92	49.619	-11.905	59.883	1.00	26.84	O
ATOM	3227	CB	GLU	C	92	51.203	-14.259	61.626	1.00	29.91	C
ATOM	3228	CG	GLU	C	92	52.383	-13.725	62.416	1.00	31.69	C

FIG. 53-54

ATOM	3230	OE1	GLU	C	92	54.115	-14.880	61.230	1.00	34.93	O
ATOM	3231	OE2	GLU	C	92	54.013	-15.165	63.409	1.00	32.07	O
ATOM	3232	N	VAL	C	93	50.683	-11.147	61.726	1.00	25.33	N
ATOM	3233	CA	VAL	C	93	50.925	-9.806	61.189	1.00	23.43	C
ATOM	3234	C	VAL	C	93	52.093	-9.083	61.875	1.00	22.86	C
ATOM	3235	O	VAL	C	93	52.321	-9.234	63.070	1.00	22.87	O
ATOM	3236	CB	VAL	C	93	49.651	-8.914	61.251	1.00	22.01	C
ATOM	3237	CG1	VAL	C	93	49.281	-8.588	62.678	1.00	21.69	C
ATOM	3238	CG2	VAL	C	93	49.857	-7.644	60.453	1.00	20.43	C
ATOM	3239	N	GLN	C	94	52.859	-8.330	61.098	1.00	24.05	N
ATOM	3240	CA	GLN	C	94	53.986	-7.581	61.626	1.00	24.23	C
ATOM	3241	C	GLN	C	94	53.602	-6.110	61.602	1.00	24.03	C
ATOM	3242	O	GLN	C	94	53.295	-5.554	60.543	1.00	23.15	O
ATOM	3243	CB	GLN	C	94	55.219	-7.823	60.765	1.00	27.34	C
ATOM	3244	CG	GLN	C	94	56.502	-7.267	61.340	1.00	29.54	C
ATOM	3245	CD	GLN	C	94	57.719	-7.813	60.629	1.00	30.13	C
ATOM	3246	OE1	GLN	C	94	58.107	-7.317	59.575	1.00	29.70	O
ATOM	3247	NE2	GLN	C	94	58.316	-8.857	61.193	1.00	30.59	N
ATOM	3248	N	LEU	C	95	53.579	-5.498	62.782	1.00	22.86	N
ATOM	3249	CA	LEU	C	95	53.205	-4.097	62.922	1.00	19.68	C
ATOM	3250	C	LEU	C	95	54.424	-3.258	63.276	1.00	17.31	C
ATOM	3251	O	LEU	C	95	55.025	-3.449	64.337	1.00	18.01	O
ATOM	3252	CB	LEU	C	95	52.114	-3.959	63.995	1.00	19.68	C
ATOM	3253	CG	LEU	C	95	51.338	-2.647	64.196	1.00	19.09	C
ATOM	3254	CD1	LEU	C	95	51.960	-1.830	65.312	1.00	19.14	C
ATOM	3255	CD2	LEU	C	95	51.231	-1.856	62.887	1.00	18.25	C
ATOM	3256	N	LEU	C	96	54.818	-2.385	62.351	1.00	15.00	N
ATOM	3257	CA	LEU	C	96	55.958	-1.486	62.533	1.00	14.64	C
ATOM	3258	C	LEU	C	96	55.464	-0.058	62.726	1.00	14.32	C
ATOM	3259	O	LEU	C	96	54.757	0.462	61.870	1.00	13.77	O
ATOM	3260	CB	LEU	C	96	56.872	-1.502	61.301	1.00	12.86	C
ATOM	3261	CG	LEU	C	96	57.840	-2.651	61.021	1.00	11.86	C
ATOM	3262	CD1	LEU	C	96	58.845	-2.759	62.140	1.00	10.73	C
ATOM	3263	CD2	LEU	C	96	57.093	-3.957	60.830	1.00	13.07	C
ATOM	3264	N	VAL	C	97	55.830	0.580	63.832	1.00	15.46	N
ATOM	3265	CA	VAL	C	97	55.412	1.964	64.056	1.00	17.77	C
ATOM	3266	C	VAL	C	97	56.549	2.929	63.755	1.00	19.55	C
ATOM	3267	O	VAL	C	97	57.657	2.775	64.276	1.00	20.22	O
ATOM	3268	CB	VAL	C	97	54.908	2.213	65.483	1.00	16.29	C
ATOM	3269	CG1	VAL	C	97	54.597	3.676	65.659	1.00	15.45	C
ATOM	3270	CG2	VAL	C	97	53.655	1.391	65.743	1.00	18.13	C
ATOM	3271	N	PHE	C	98	56.262	3.934	62.931	1.00	20.93	N
ATOM	3272	CA	PHE	C	98	57.276	4.909	62.548	1.00	21.36	C
ATOM	3273	C	PHE	C	98	56.982	6.307	63.032	1.00	22.58	C
ATOM	3274	O	PHE	C	98	55.821	6.713	63.147	1.00	22.72	O
ATOM	3275	CB	PHE	C	98	57.435	4.942	61.029	1.00	19.80	C
ATOM	3276	CG	PHE	C	98	58.015	3.688	60.455	1.00	15.93	C
ATOM	3277	CD1	PHE	C	98	59.359	3.385	60.640	1.00	12.64	C
ATOM	3278	CD2	PHE	C	98	57.217	2.814	59.730	1.00	13.16	C
ATOM	3279	CE1	PHE	C	98	59.898	2.228	60.110	1.00	15.16	C
ATOM	3280	CE2	PHE	C	98	57.745	1.657	59.198	1.00	13.93	C
ATOM	3281	CZ	PHE	C	98	59.087	1.358	59.384	1.00	14.61	C
ATOM	3282	N	GLY	C	99	58.058	7.044	63.285	1.00	23.57	N
ATOM	3283	CA	GLY	C	99	57.958	8.421	63.733	1.00	23.82	C
ATOM	3284	C	GLY	C	99	58.810	9.247	62.793	1.00	22.91	C
ATOM	3285	O	GLY	C	99	59.772	8.736	62.208	1.00	23.10	O
ATOM	3286	N	LEU	C	100	58.448	10.510	62.619	1.00	22.42	N
ATOM	3287	CA	LEU	C	100	59.184	11.398	61.729	1.00	21.39	C
ATOM	3288	C	LEU	C	100	59.049	12.812	62.271	1.00	22.04	C
ATOM	3289	O	LEU	C	100	58.090	13.519	61.969	1.00	21.68	O
ATOM	3290	CB	LEU	C	100	58.606	11.287	60.312	1.00	20.03	C
ATOM	3291	CG	LEU	C	100	59.312	11.872	59.089	1.00	17.21	C
ATOM	3292	CD1	LEU	C	100	58.976	13.336	58.940	1.00	18.15	C
ATOM	3293	CD2	LEU	C	100	60.810	11.635	59.176	1.00	16.63	C
ATOM	3294	N	THR	C	101	59.985	13.199	63.124	1.00	23.11	N
ATOM	3295	CA	THR	C	101	59.951	14.528	63.717	1.00	24.58	C
ATOM	3296	C	THR	C	101	60.973	15.503	63.142	1.00	25.44	C
ATOM	3297	O	THR	C	101	62.166	15.189	63.036	1.00	24.67	O
ATOM	3298	CB	THR	C	101	60.111	14.460	65.254	1.00	23.29	C
ATOM	3299	OG1	THR	C	101	61.249	13.654	65.594	1.00	21.98	O

FIG. 53-55

ATOM	3301	N	ALA	C	102	60.485	16.670	62.733	1.00	27.01	N
ATOM	3302	CA	ALA	C	102	61.345	17.719	62.199	1.00	29.09	C
ATOM	3303	C	ALA	C	102	62.055	18.372	63.388	1.00	30.36	C
ATOM	3304	O	ALA	C	102	61.405	18.913	64.289	1.00	29.10	O
ATOM	3305	CB	ALA	C	102	60.514	18.749	61.431	1.00	27.84	C
ATOM	3306	N	ASN	C	103	63.377	18.241	63.421	1.00	32.41	N
ATOM	3307	CA	ASN	C	103	64.196	18.803	64.492	1.00	34.64	C
ATOM	3308	C	ASN	C	103	64.144	20.316	64.424	1.00	37.19	C
ATOM	3309	O	ASN	C	103	64.032	21.000	65.446	1.00	37.42	O
ATOM	3310	CB	ASN	C	103	65.667	18.378	64.349	1.00	32.99	C
ATOM	3311	CG	ASN	C	103	65.842	16.893	64.091	1.00	31.59	C
ATOM	3312	OD1	ASN	C	103	64.895	16.187	63.752	1.00	30.54	O
ATOM	3313	ND2	ASN	C	103	67.074	16.419	64.211	1.00	30.79	N
ATOM	3314	N	SER	C	104	64.192	20.829	63.200	1.00	39.57	N
ATOM	3315	CA	SER	C	104	64.200	22.264	62.938	1.00	41.79	C
ATOM	3316	C	SER	C	104	62.930	23.056	63.245	1.00	42.49	C
ATOM	3317	O	SER	C	104	62.711	24.110	62.640	1.00	43.24	O
ATOM	3318	CB	SER	C	104	64.606	22.493	61.486	1.00	41.64	C
ATOM	3319	OG	SER	C	104	65.582	21.542	61.099	1.00	43.50	O
ATOM	3320	N	ASP	C	105	62.112	22.584	64.187	1.00	42.26	N
ATOM	3321	CA	ASP	C	105	60.879	23.291	64.534	1.00	42.59	C
ATOM	3322	C	ASP	C	105	60.088	23.535	63.233	1.00	41.49	C
ATOM	3323	O	ASP	C	105	59.841	22.597	62.463	1.00	40.81	O
ATOM	3324	CB	ASP	C	105	61.221	24.619	65.266	1.00	44.61	C
ATOM	3325	CG	ASP	C	105	59.983	25.449	65.632	1.00	45.96	C
ATOM	3326	OD1	ASP	C	105	59.109	24.940	66.360	1.00	47.35	O
ATOM	3327	OD2	ASP	C	105	59.883	26.612	65.171	1.00	44.21	O
ATOM	3328	N	THR	C	106	59.742	24.794	62.971	1.00	39.76	N
ATOM	3329	CA	THR	C	106	59.001	25.195	61.789	1.00	37.14	C
ATOM	3330	C	THR	C	106	59.419	26.626	61.483	1.00	35.28	C
ATOM	3331	O	THR	C	106	59.939	26.889	60.400	1.00	36.37	O
ATOM	3332	CB	THR	C	106	57.452	25.137	61.985	1.00	37.13	C
ATOM	3333	OG1	THR	C	106	57.028	26.127	62.939	1.00	40.63	O
ATOM	3334	CG2	THR	C	106	57.010	23.763	62.449	1.00	36.75	C
ATOM	3335	N	HIS	C	107	59.241	27.529	62.451	1.00	32.22	N
ATOM	3336	CA	HIS	C	107	59.589	28.946	62.281	1.00	28.91	C
ATOM	3337	C	HIS	C	107	61.092	29.188	62.167	1.00	25.62	C
ATOM	3338	O	HIS	C	107	61.747	29.544	63.147	1.00	25.53	O
ATOM	3339	CB	HIS	C	107	59.049	29.780	63.439	1.00	29.99	C
ATOM	3340	CG	HIS	C	107	57.633	30.230	63.266	1.00	33.11	C
ATOM	3341	ND1	HIS	C	107	56.552	29.421	63.556	1.00	34.87	N
ATOM	3342	CD2	HIS	C	107	57.117	31.431	62.911	1.00	33.23	C
ATOM	3343	CE1	HIS	C	107	55.435	30.108	63.394	1.00	34.92	C
ATOM	3344	NE2	HIS	C	107	55.749	31.331	63.001	1.00	34.15	N
ATOM	3345	N	LEU	C	108	61.631	29.011	60.968	1.00	22.10	N
ATOM	3346	CA	LEU	C	108	63.050	29.207	60.725	1.00	18.56	C
ATOM	3347	C	LEU	C	108	63.240	30.371	59.778	1.00	16.16	C
ATOM	3348	O	LEU	C	108	62.281	30.923	59.255	1.00	16.77	O
ATOM	3349	CB	LEU	C	108	63.664	27.953	60.092	1.00	17.86	C
ATOM	3350	CG	LEU	C	108	63.637	26.645	60.880	1.00	17.69	C
ATOM	3351	CD1	LEU	C	108	63.980	25.503	59.969	1.00	18.79	C
ATOM	3352	CD2	LEU	C	108	64.612	26.702	62.026	1.00	19.44	C
ATOM	3353	N	LEU	C	109	64.496	30.716	59.537	1.00	14.36	N
ATOM	3354	CA	LEU	C	109	64.860	31.807	58.641	1.00	13.06	C
ATOM	3355	C	LEU	C	109	65.400	31.265	57.309	1.00	13.45	C
ATOM	3356	O	LEU	C	109	65.966	30.165	57.247	1.00	14.08	O
ATOM	3357	CB	LEU	C	109	65.933	32.682	59.306	1.00	10.18	C
ATOM	3358	CG	LEU	C	109	65.532	33.727	60.358	1.00	8.93	C
ATOM	3359	CD1	LEU	C	109	64.219	33.398	61.045	1.00	7.76	C
ATOM	3360	CD2	LEU	C	109	66.656	33.883	61.362	1.00	7.47	C
ATOM	3361	N	GLN	C	110	65.217	32.029	56.238	1.00	13.10	N
ATOM	3362	CA	GLN	C	110	65.728	31.617	54.944	1.00	13.18	C
ATOM	3363	C	GLN	C	110	67.235	31.434	55.148	1.00	12.96	C
ATOM	3364	O	GLN	C	110	67.888	32.272	55.777	1.00	13.50	O
ATOM	3365	CB	GLN	C	110	65.456	32.695	53.897	1.00	13.63	C
ATOM	3366	CG	GLN	C	110	63.999	33.126	53.822	1.00	14.21	C
ATOM	3367	CD	GLN	C	110	63.728	34.044	52.649	1.00	14.20	C
ATOM	3368	OE1	GLN	C	110	64.558	34.173	51.746	1.00	17.32	O
ATOM	3369	NE2	GLN	C	110	62.563	34.671	52.642	1.00	14.14	N
ATOM	3370	N	GLY	C	111	67.781	30.331	54.650	1.00	11.64	N

FIG. 53-56

ATOM	3372	C	GLY	C	111	69.411	29.082	55.965	1.00	9.44	C
ATOM	3373	O	GLY	C	111	70.521	28.591	56.172	1.00	7.92	O
ATOM	3374	N	GLN	C	112	68.348	28.797	56.715	1.00	8.64	N
ATOM	3375	CA	GLN	C	112	68.431	27.854	57.821	1.00	9.62	C
ATOM	3376	C	GLN	C	112	68.185	26.398	57.429	1.00	10.09	C
ATOM	3377	O	GLN	C	112	67.370	26.101	56.548	1.00	8.32	O
ATOM	3378	CB	GLN	C	112	67.503	28.274	58.945	1.00	9.21	C
ATOM	3379	CG	GLN	C	112	68.252	28.942	60.053	1.00	9.18	C
ATOM	3380	CD	GLN	C	112	67.408	29.901	60.831	1.00	8.46	C
ATOM	3381	OE1	GLN	C	112	67.772	31.061	60.980	1.00	10.11	O
ATOM	3382	NE2	GLN	C	112	66.280	29.431	61.344	1.00	8.06	N
ATOM	3383	N	SER	C	113	68.890	25.497	58.106	1.00	9.99	N
ATOM	3384	CA	SER	C	113	68.793	24.072	57.832	1.00	9.32	C
ATOM	3385	C	SER	C	113	67.532	23.443	58.361	1.00	9.91	C
ATOM	3386	O	SER	C	113	66.925	23.938	59.300	1.00	10.90	O
ATOM	3387	CB	SER	C	113	69.971	23.345	58.448	1.00	7.24	C
ATOM	3388	OG	SER	C	113	71.197	24.002	58.179	1.00	10.17	O
ATOM	3389	N	LEU	C	114	67.148	22.337	57.747	1.00	10.93	N
ATOM	3390	CA	LEU	C	114	65.972	21.587	58.157	1.00	9.91	C
ATOM	3391	C	LEU	C	114	66.532	20.203	58.413	1.00	9.55	C
ATOM	3392	O	LEU	C	114	67.512	19.807	57.778	1.00	10.78	O
ATOM	3393	CB	LEU	C	114	64.943	21.557	57.030	1.00	9.40	C
ATOM	3394	CG	LEU	C	114	63.558	20.933	57.208	1.00	9.41	C
ATOM	3395	CD1	LEU	C	114	63.611	19.422	57.055	1.00	11.32	C
ATOM	3396	CD2	LEU	C	114	62.964	21.329	58.524	1.00	8.77	C
ATOM	3397	N	THR	C	115	65.981	19.506	59.394	1.00	10.23	N
ATOM	3398	CA	THR	C	115	66.428	18.157	59.710	1.00	11.34	C
ATOM	3399	C	THR	C	115	65.248	17.340	60.211	1.00	12.00	C
ATOM	3400	O	THR	C	115	64.516	17.773	61.094	1.00	12.84	O
ATOM	3401	CB	THR	C	115	67.560	18.162	60.760	1.00	11.32	C
ATOM	3402	OG1	THR	C	115	68.714	18.828	60.231	1.00	13.64	O
ATOM	3403	CG2	THR	C	115	67.957	16.758	61.126	1.00	12.70	C
ATOM	3404	N	LEU	C	116	65.021	16.203	59.568	1.00	14.83	N
ATOM	3405	CA	LEU	C	116	63.938	15.286	59.920	1.00	17.05	C
ATOM	3406	C	LEU	C	116	64.579	14.013	60.466	1.00	17.08	C
ATOM	3407	O	LEU	C	116	65.514	13.483	59.861	1.00	16.50	O
ATOM	3408	CB	LEU	C	116	63.105	14.951	58.676	1.00	19.24	C
ATOM	3409	CG	LEU	C	116	62.368	16.126	58.024	1.00	22.16	C
ATOM	3410	CD1	LEU	C	116	61.885	15.728	56.663	1.00	24.14	C
ATOM	3411	CD2	LEU	C	116	61.201	16.561	58.888	1.00	23.58	C
ATOM	3412	N	THR	C	117	64.111	13.559	61.626	1.00	17.08	N
ATOM	3413	CA	THR	C	117	64.644	12.357	62.248	1.00	17.55	C
ATOM	3414	C	THR	C	117	63.606	11.247	62.186	1.00	18.51	C
ATOM	3415	O	THR	C	117	62.416	11.463	62.444	1.00	18.03	O
ATOM	3416	CB	THR	C	117	65.050	12.606	63.720	1.00	18.69	C
ATOM	3417	OG1	THR	C	117	65.874	13.773	63.803	1.00	19.51	O
ATOM	3418	CG2	THR	C	117	65.837	11.417	64.269	1.00	18.84	C
ATOM	3419	N	LEU	C	118	64.068	10.065	61.800	1.00	20.36	N
ATOM	3420	CA	LEU	C	118	63.223	8.891	61.683	1.00	21.54	C
ATOM	3421	C	LEU	C	118	63.245	8.114	62.989	1.00	23.23	C
ATOM	3422	O	LEU	C	118	64.313	7.700	63.449	1.00	23.33	O
ATOM	3423	CB	LEU	C	118	63.751	7.998	60.561	1.00	21.86	C
ATOM	3424	CG	LEU	C	118	62.976	6.721	60.224	1.00	22.93	C
ATOM	3425	CD1	LEU	C	118	61.767	7.052	59.348	1.00	20.94	C
ATOM	3426	CD2	LEU	C	118	63.909	5.754	59.516	1.00	23.45	C
ATOM	3427	N	GLU	C	119	62.079	7.960	63.608	1.00	25.58	N
ATOM	3428	CA	GLU	C	119	61.961	7.198	64.849	1.00	28.53	C
ATOM	3429	C	GLU	C	119	61.478	5.813	64.409	1.00	30.40	C
ATOM	3430	O	GLU	C	119	60.285	5.595	64.163	1.00	30.34	O
ATOM	3431	CB	GLU	C	119	60.960	7.858	65.798	1.00	28.11	C
ATOM	3432	CG	GLU	C	119	61.094	7.425	67.252	1.00	29.88	C
ATOM	3433	CD	GLU	C	119	60.427	8.391	68.222	1.00	32.15	C
ATOM	3434	OE1	GLU	C	119	59.438	9.056	67.845	1.00	32.83	O
ATOM	3435	OE2	GLU	C	119	60.902	8.510	69.366	1.00	34.00	O
ATOM	3436	N	SER	C	120	62.431	4.906	64.231	1.00	31.45	N
ATOM	3437	CA	SER	C	120	62.137	3.556	63.775	1.00	31.95	C
ATOM	3438	C	SER	C	120	62.286	2.504	64.869	1.00	31.72	C
ATOM	3439	O	SER	C	120	63.079	2.677	65.806	1.00	31.27	O
ATOM	3440	CB	SER	C	120	63.055	3.207	62.595	1.00	33.02	C
ATOM	3441	OG	SER	C	120	64.428	3.278	62.964	1.00	35.08	O

FIG. 53-57

ATOM	3443	CA	PRO	C	121	61.528	0.276	65.702	1.00	32.79	C
ATOM	3444	C	PRO	C	121	62.739	-0.637	65.541	1.00	33.59	C
ATOM	3445	O	PRO	C	121	63.454	-0.578	64.537	1.00	34.27	O
ATOM	3446	CB	PRO	C	121	60.244	-0.463	65.344	1.00	32.32	C
ATOM	3447	CG	PRO	C	121	60.123	-0.223	63.882	1.00	31.58	C
ATOM	3448	CD	PRO	C	121	60.439	1.239	63.775	1.00	30.99	C
ATOM	3449	N	PRO	C	122	63.020	-1.457	66.560	1.00	34.59	N
ATOM	3450	CA	PRO	C	122	64.146	-2.391	66.541	1.00	36.28	C
ATOM	3451	C	PRO	C	122	64.024	-3.473	65.463	1.00	36.86	C
ATOM	3452	O	PRO	C	122	63.143	-4.330	65.532	1.00	37.23	O
ATOM	3453	CB	PRO	C	122	64.098	-2.998	67.943	1.00	37.24	C
ATOM	3454	CG	PRO	C	122	63.611	-1.862	68.772	1.00	36.95	C
ATOM	3455	CD	PRO	C	122	62.465	-1.345	67.921	1.00	36.11	C
ATOM	3456	N	GLY	C	123	64.902	-3.415	64.465	1.00	37.07	N
ATOM	3457	CA	GLY	C	123	64.884	-4.406	63.405	1.00	38.07	C
ATOM	3458	C	GLY	C	123	64.528	-3.924	62.010	1.00	38.76	C
ATOM	3459	O	GLY	C	123	64.528	-4.725	61.071	1.00	38.36	O
ATOM	3460	N	SER	C	124	64.244	-2.632	61.851	1.00	39.57	N
ATOM	3461	CA	SER	C	124	63.878	-2.095	60.544	1.00	40.33	C
ATOM	3462	C	SER	C	124	64.870	-1.078	59.995	1.00	41.01	C
ATOM	3463	O	SER	C	124	65.420	-0.270	60.751	1.00	41.37	O
ATOM	3464	CB	SER	C	124	62.487	-1.462	60.608	1.00	39.66	C
ATOM	3465	OG	SER	C	124	62.434	-0.456	61.606	1.00	39.35	O
ATOM	3466	N	SER	C	125	65.060	-1.111	58.677	1.00	40.58	N
ATOM	3467	CA	SER	C	125	65.951	-0.195	57.965	1.00	40.60	C
ATOM	3468	C	SER	C	125	65.177	0.236	56.718	1.00	39.94	C
ATOM	3469	O	SER	C	125	65.263	-0.411	55.670	1.00	40.98	O
ATOM	3470	CB	SER	C	125	67.242	-0.916	57.551	1.00	41.65	C
ATOM	3471	OG	SER	C	125	67.889	-1.526	58.657	1.00	42.74	O
ATOM	3472	N	PRO	C	126	64.378	1.312	56.824	1.00	39.20	N
ATOM	3473	CA	PRO	C	126	63.585	1.805	55.697	1.00	38.71	C
ATOM	3474	C	PRO	C	126	64.209	2.964	54.926	1.00	38.11	C
ATOM	3475	O	PRO	C	126	65.289	3.439	55.270	1.00	37.95	O
ATOM	3476	CB	PRO	C	126	62.304	2.243	56.389	1.00	38.90	C
ATOM	3477	CG	PRO	C	126	62.837	2.909	57.622	1.00	38.15	C
ATOM	3478	CD	PRO	C	126	63.986	2.000	58.071	1.00	39.42	C
ATOM	3479	N	SER	C	127	63.521	3.401	53.875	1.00	37.81	N
ATOM	3480	CA	SER	C	127	63.972	4.528	53.062	1.00	38.14	C
ATOM	3481	C	SER	C	127	62.956	5.661	53.161	1.00	38.67	C
ATOM	3482	O	SER	C	127	61.754	5.437	53.026	1.00	39.41	O
ATOM	3483	CB	SER	C	127	64.170	4.114	51.602	1.00	37.77	C
ATOM	3484	OG	SER	C	127	65.456	3.535	51.401	1.00	38.00	O
ATOM	3485	N	VAL	C	128	63.453	6.873	53.384	1.00	38.92	N
ATOM	3486	CA	VAL	C	128	62.616	8.061	53.543	1.00	38.70	C
ATOM	3487	C	VAL	C	128	62.735	8.998	52.341	1.00	38.75	C
ATOM	3488	O	VAL	C	128	63.798	9.103	51.717	1.00	38.09	O
ATOM	3489	CB	VAL	C	128	63.011	8.858	54.814	1.00	38.43	C
ATOM	3490	CG1	VAL	C	128	61.945	9.881	55.148	1.00	37.66	C
ATOM	3491	CG2	VAL	C	128	63.243	7.921	55.995	1.00	38.66	C
ATOM	3492	N	GLN	C	129	61.644	9.705	52.051	1.00	38.20	N
ATOM	3493	CA	GLN	C	129	61.580	10.649	50.936	1.00	37.25	C
ATOM	3494	C	GLN	C	129	60.685	11.814	51.334	1.00	35.80	C
ATOM	3495	O	GLN	C	129	59.489	11.629	51.574	1.00	35.49	O
ATOM	3496	CB	GLN	C	129	61.018	9.951	49.687	1.00	38.46	C
ATOM	3497	CG	GLN	C	129	60.652	10.861	48.511	1.00	41.45	C
ATOM	3498	CD	GLN	C	129	59.143	11.067	48.350	1.00	43.36	C
ATOM	3499	OE1	GLN	C	129	58.334	10.276	48.843	1.00	43.93	O
ATOM	3500	NE2	GLN	C	129	58.763	12.130	47.648	1.00	41.25	N
ATOM	3501	N	CYS	C	130	61.270	13.000	51.456	1.00	34.06	N
ATOM	3502	CA	CYS	C	130	60.501	14.183	51.817	1.00	32.97	C
ATOM	3503	C	CYS	C	130	60.526	15.161	50.660	1.00	31.87	C
ATOM	3504	O	CYS	C	130	61.581	15.415	50.081	1.00	31.95	O
ATOM	3505	CB	CYS	C	130	61.075	14.859	53.063	1.00	34.29	C
ATOM	3506	SG	CYS	C	130	60.956	13.916	54.615	1.00	34.97	S
ATOM	3507	N	ARG	C	131	59.362	15.711	50.333	1.00	30.51	N
ATOM	3508	CA	ARG	C	131	59.233	16.655	49.238	1.00	28.80	C
ATOM	3509	C	ARG	C	131	58.691	17.965	49.800	1.00	27.51	C
ATOM	3510	O	ARG	C	131	57.660	17.982	50.475	1.00	26.63	O
ATOM	3511	CB	ARG	C	131	58.277	16.085	48.190	1.00	29.85	C
ATOM	3512	CG	ARG	C	131	58.232	16.829	46.877	1.00	32.22	C

FIG. 53-58

ATOM	3514	NE	ARG	C	131	58.861	16.759	44.505	1.00	38.86	N
ATOM	3515	CZ	ARG	C	131	59.210	16.182	43.357	1.00	40.02	C
ATOM	3516	NH1	ARG	C	131	59.868	15.028	43.361	1.00	40.08	N
ATOM	3517	NH2	ARG	C	131	58.880	16.751	42.202	1.00	39.80	N
ATOM	3518	N	SER	C	132	59.417	19.049	49.549	1.00	25.96	N
ATOM	3519	CA	SER	C	132	59.045	20.383	50.013	1.00	24.47	C
ATOM	3520	C	SER	C	132	57.892	20.928	49.185	1.00	23.51	C
ATOM	3521	O	SER	C	132	57.597	20.409	48.105	1.00	24.24	O
ATOM	3522	CB	SER	C	132	60.235	21.332	49.873	1.00	23.44	C
ATOM	3523	OG	SER	C	132	60.485	21.586	48.506	1.00	20.32	O
ATOM	3524	N	PRO	C	133	57.258	22.018	49.647	1.00	22.71	N
ATOM	3525	CA	PRO	C	133	56.141	22.608	48.909	1.00	21.46	C
ATOM	3526	C	PRO	C	133	56.516	22.930	47.464	1.00	21.15	C
ATOM	3527	O	PRO	C	133	55.660	22.899	46.585	1.00	21.36	O
ATOM	3528	CB	PRO	C	133	55.849	23.868	49.711	1.00	19.38	C
ATOM	3529	CG	PRO	C	133	56.170	23.441	51.096	1.00	18.92	C
ATOM	3530	CD	PRO	C	133	57.470	22.733	50.917	1.00	21.34	C
ATOM	3531	N	ARG	C	134	57.797	23.222	47.224	1.00	21.78	N
ATOM	3532	CA	ARG	C	134	58.285	23.541	45.878	1.00	21.34	C
ATOM	3533	C	ARG	C	134	58.969	22.372	45.150	1.00	21.00	C
ATOM	3534	O	ARG	C	134	59.787	22.569	44.251	1.00	21.10	O
ATOM	3535	CB	ARG	C	134	59.183	24.788	45.893	1.00	20.36	C
ATOM	3536	CG	ARG	C	134	60.260	24.810	46.968	1.00	21.80	C
ATOM	3537	CD	ARG	C	134	61.635	24.362	46.458	1.00	24.10	C
ATOM	3538	NE	ARG	C	134	62.653	24.468	47.507	1.00	24.28	N
ATOM	3539	CZ	ARG	C	134	63.968	24.506	47.306	1.00	24.06	C
ATOM	3540	NH1	ARG	C	134	64.473	24.444	46.084	1.00	24.86	N
ATOM	3541	NH2	ARG	C	134	64.775	24.674	48.339	1.00	26.77	N
ATOM	3542	N	GLY	C	135	58.621	21.150	45.537	1.00	20.48	N
ATOM	3543	CA	GLY	C	135	59.185	19.978	44.892	1.00	17.34	C
ATOM	3544	C	GLY	C	135	60.623	19.629	45.222	1.00	15.25	C
ATOM	3545	O	GLY	C	135	61.174	18.715	44.616	1.00	15.64	O
ATOM	3546	N	LYS	C	136	61.247	20.364	46.136	1.00	13.71	N
ATOM	3547	CA	LYS	C	136	62.625	20.072	46.536	1.00	13.59	C
ATOM	3548	C	LYS	C	136	62.572	18.805	47.398	1.00	13.78	C
ATOM	3549	O	LYS	C	136	61.961	18.813	48.464	1.00	12.87	O
ATOM	3550	CB	LYS	C	136	63.207	21.257	47.335	1.00	13.17	C
ATOM	3551	CG	LYS	C	136	64.350	20.921	48.304	1.00	11.86	C
ATOM	3552	CD	LYS	C	136	65.713	21.282	47.752	1.00	8.91	C
ATOM	3553	CE	LYS	C	136	66.821	20.647	48.565	1.00	9.07	C
ATOM	3554	NZ	LYS	C	136	66.698	19.152	48.557	1.00	12.43	N
ATOM	3555	N	ASN	C	137	63.173	17.712	46.938	1.00	15.38	N
ATOM	3556	CA	ASN	C	137	63.130	16.487	47.728	1.00	16.86	C
ATOM	3557	C	ASN	C	137	64.450	16.008	48.325	1.00	16.82	C
ATOM	3558	O	ASN	C	137	65.529	16.277	47.801	1.00	16.16	O
ATOM	3559	CB	ASN	C	137	62.399	15.354	46.988	1.00	19.19	C
ATOM	3560	CG	ASN	C	137	63.016	15.023	45.649	1.00	21.52	C
ATOM	3561	OD1	ASN	C	137	62.582	15.540	44.604	1.00	21.42	O
ATOM	3562	ND2	ASN	C	137	63.998	14.119	45.652	1.00	22.72	N
ATOM	3563	N	ILE	C	138	64.341	15.381	49.488	1.00	17.42	N
ATOM	3564	CA	ILE	C	138	65.479	14.854	50.227	1.00	17.65	C
ATOM	3565	C	ILE	C	138	65.213	13.366	50.497	1.00	18.77	C
ATOM	3566	O	ILE	C	138	64.070	12.968	50.772	1.00	17.83	O
ATOM	3567	CB	ILE	C	138	65.695	15.651	51.540	1.00	16.36	C
ATOM	3568	CG1	ILE	C	138	64.376	15.799	52.308	1.00	16.75	C
ATOM	3569	CG2	ILE	C	138	66.221	17.040	51.213	1.00	15.86	C
ATOM	3570	CD1	ILE	C	138	64.500	16.523	53.648	1.00	15.58	C
ATOM	3571	N	GLN	C	139	66.262	12.552	50.375	1.00	19.50	N
ATOM	3572	CA	GLN	C	139	66.157	11.108	50.556	1.00	21.45	C
ATOM	3573	C	GLN	C	139	67.162	10.595	51.571	1.00	21.93	C
ATOM	3574	O	GLN	C	139	68.333	10.949	51.509	1.00	23.09	O
ATOM	3575	CB	GLN	C	139	66.363	10.374	49.219	1.00	23.24	C
ATOM	3576	CG	GLN	C	139	66.679	11.249	47.986	1.00	27.09	C
ATOM	3577	CD	GLN	C	139	68.030	11.970	48.048	1.00	29.61	C
ATOM	3578	OE1	GLN	C	139	68.177	13.075	47.520	1.00	28.85	O
ATOM	3579	NE2	GLN	C	139	69.014	11.353	48.690	1.00	30.92	N
ATOM	3580	N	GLY	C	140	66.712	9.743	52.484	1.00	22.40	N
ATOM	3581	CA	GLY	C	140	67.603	9.202	53.499	1.00	24.32	C
ATOM	3582	C	GLY	C	140	66.971	8.072	54.297	1.00	25.45	C
ATOM	3583	O	GLY	C	140	65.848	7.662	54.002	1.00	25.77	O

FIG. 53-59

ATOM	3585	CA	GLY	C	141	67.098	6.508	56.119	1.00	24.09	C
ATOM	3586	C	GLY	C	141	67.280	6.660	57.613	1.00	24.16	C
ATOM	3587	O	GLY	C	141	67.559	5.690	58.317	1.00	25.48	O
ATOM	3588	N	LYS	C	142	67.118	7.882	58.097	1.00	23.81	N
ATOM	3589	CA	LYS	C	142	67.259	8.190	59.512	1.00	23.83	C
ATOM	3590	C	LYS	C	142	67.099	9.701	59.623	1.00	23.09	C
ATOM	3591	O	LYS	C	142	66.019	10.199	59.942	1.00	22.51	O
ATOM	3592	CB	LYS	C	142	68.634	7.752	60.044	1.00	24.56	C
ATOM	3593	CG	LYS	C	142	68.791	7.800	61.572	1.00	27.42	C
ATOM	3594	CD	LYS	C	142	68.575	6.433	62.239	1.00	25.14	C
ATOM	3595	CE	LYS	C	142	67.124	5.972	62.149	1.00	27.04	C
ATOM	3596	NZ	LYS	C	142	66.894	4.599	62.699	1.00	27.76	N
ATOM	3597	N	THR	C	143	68.146	10.433	59.271	1.00	21.45	N
ATOM	3598	CA	THR	C	143	68.074	11.874	59.348	1.00	20.52	C
ATOM	3599	C	THR	C	143	68.160	12.497	57.965	1.00	20.63	C
ATOM	3600	O	THR	C	143	69.124	12.279	57.233	1.00	20.70	O
ATOM	3601	CB	THR	C	143	69.150	12.455	60.295	1.00	20.16	C
ATOM	3602	OG1	THR	C	143	68.901	13.850	60.504	1.00	22.12	O
ATOM	3603	CG2	THR	C	143	70.558	12.259	59.737	1.00	17.82	C
ATOM	3604	N	LEU	C	144	67.093	13.170	57.565	1.00	20.19	N
ATOM	3605	CA	LEU	C	144	67.083	13.839	56.280	1.00	19.88	C
ATOM	3606	C	LEU	C	144	67.425	15.298	56.533	1.00	20.01	C
ATOM	3607	O	LEU	C	144	67.055	15.877	57.565	1.00	18.86	O
ATOM	3608	CB	LEU	C	144	65.725	13.721	55.587	1.00	19.27	C
ATOM	3609	CG	LEU	C	144	65.468	12.475	54.744	1.00	17.79	C
ATOM	3610	CD1	LEU	C	144	65.432	11.262	55.631	1.00	17.30	C
ATOM	3611	CD2	LEU	C	144	64.148	12.627	54.018	1.00	17.18	C
ATOM	3612	N	SER	C	145	68.153	15.891	55.602	1.00	19.94	N
ATOM	3613	CA	SER	C	145	68.533	17.273	55.762	1.00	20.38	C
ATOM	3614	C	SER	C	145	68.385	18.092	54.492	1.00	20.97	C
ATOM	3615	O	SER	C	145	68.109	17.562	53.411	1.00	22.10	O
ATOM	3616	CB	SER	C	145	69.972	17.351	56.259	1.00	18.81	C
ATOM	3617	OG	SER	C	145	70.087	16.818	57.558	1.00	14.54	O
ATOM	3618	N	VAL	C	146	68.515	19.400	54.677	1.00	19.20	N
ATOM	3619	CA	VAL	C	146	68.462	20.405	53.628	1.00	17.60	C
ATOM	3620	C	VAL	C	146	69.337	21.460	54.287	1.00	18.03	C
ATOM	3621	O	VAL	C	146	68.974	21.994	55.345	1.00	18.89	O
ATOM	3622	CB	VAL	C	146	67.055	21.002	53.461	1.00	16.34	C
ATOM	3623	CG1	VAL	C	146	67.002	21.849	52.211	1.00	16.62	C
ATOM	3624	CG2	VAL	C	146	65.996	19.913	53.420	1.00	16.04	C
ATOM	3625	N	SER	C	147	70.531	21.681	53.743	1.00	17.43	N
ATOM	3626	CA	SER	C	147	71.447	22.658	54.329	1.00	15.43	C
ATOM	3627	C	SER	C	147	70.859	24.070	54.415	1.00	13.97	C
ATOM	3628	O	SER	C	147	70.756	24.631	55.502	1.00	12.41	O
ATOM	3629	CB	SER	C	147	72.792	22.655	53.587	1.00	16.46	C
ATOM	3630	OG	SER	C	147	72.644	22.912	52.196	1.00	17.35	O
ATOM	3631	N	GLN	C	148	70.466	24.630	53.276	1.00	13.00	N
ATOM	3632	CA	GLN	C	148	69.890	25.969	53.232	1.00	11.88	C
ATOM	3633	C	GLN	C	148	68.450	25.897	52.755	1.00	9.40	C
ATOM	3634	O	GLN	C	148	68.160	25.281	51.745	1.00	10.44	O
ATOM	3635	CB	GLN	C	148	70.704	26.893	52.309	1.00	12.05	C
ATOM	3636	CG	GLN	C	148	70.103	28.301	52.175	1.00	17.81	C
ATOM	3637	CD	GLN	C	148	70.838	29.218	51.190	1.00	19.20	C
ATOM	3638	OE1	GLN	C	148	71.948	29.672	51.464	1.00	22.13	O
ATOM	3639	NE2	GLN	C	148	70.191	29.540	50.071	1.00	15.41	N
ATOM	3640	N	LEU	C	149	67.548	26.462	53.542	1.00	9.65	N
ATOM	3641	CA	LEU	C	149	66.132	26.510	53.211	1.00	8.56	C
ATOM	3642	C	LEU	C	149	65.949	27.755	52.372	1.00	10.00	C
ATOM	3643	O	LEU	C	149	66.798	28.656	52.375	1.00	9.13	O
ATOM	3644	CB	LEU	C	149	65.274	26.641	54.479	1.00	6.97	C
ATOM	3645	CG	LEU	C	149	64.448	25.444	54.966	1.00	5.33	C
ATOM	3646	CD1	LEU	C	149	65.267	24.169	54.903	1.00	7.70	C
ATOM	3647	CD2	LEU	C	149	63.960	25.700	56.376	1.00	5.54	C
ATOM	3648	N	GLU	C	150	64.811	27.823	51.702	1.00	10.94	N
ATOM	3649	CA	GLU	C	150	64.480	28.941	50.850	1.00	12.11	C
ATOM	3650	C	GLU	C	150	63.058	29.318	51.215	1.00	12.07	C
ATOM	3651	O	GLU	C	150	62.311	28.498	51.738	1.00	11.71	O
ATOM	3652	CB	GLU	C	150	64.583	28.533	49.374	1.00	14.71	C
ATOM	3653	CG	GLU	C	150	66.006	28.167	48.918	1.00	18.45	C
ATOM	3654	CD	GLU	C	150	66.951	29.372	48.877	1.00	21.09	C

FIG. 53-60

ATOM	3656	OE2	GLU	C	150	67.340	29.775	47.766	1.00	21.00	O
ATOM	3657	N	LEU	C	151	62.694	30.569	50.972	1.00	11.69	N
ATOM	3658	CA	LEU	C	151	61.365	31.052	51.293	1.00	11.57	C
ATOM	3659	C	LEU	C	151	60.289	30.112	50.790	1.00	12.44	C
ATOM	3660	O	LEU	C	151	59.308	29.851	51.494	1.00	13.93	O
ATOM	3661	CB	LEU	C	151	61.158	32.447	50.709	1.00	12.37	C
ATOM	3662	CG	LEU	C	151	59.797	33.113	50.883	1.00	13.90	C
ATOM	3663	CD1	LEU	C	151	59.406	33.231	52.352	1.00	13.05	C
ATOM	3664	CD2	LEU	C	151	59.879	34.479	50.249	1.00	16.05	C
ATOM	3665	N	GLN	C	152	60.507	29.536	49.613	1.00	12.55	N
ATOM	3666	CA	GLN	C	152	59.515	28.641	49.028	1.00	11.90	C
ATOM	3667	C	GLN	C	152	59.396	27.259	49.666	1.00	12.70	C
ATOM	3668	O	GLN	C	152	58.599	26.433	49.209	1.00	13.13	O
ATOM	3669	CB	GLN	C	152	59.707	28.529	47.519	1.00	11.46	C
ATOM	3670	CG	GLN	C	152	59.413	29.818	46.770	1.00	8.15	C
ATOM	3671	CD	GLN	C	152	60.596	30.768	46.760	1.00	9.54	C
ATOM	3672	OE1	GLN	C	152	61.649	30.483	47.339	1.00	8.38	O
ATOM	3673	NE2	GLN	C	152	60.441	31.897	46.080	1.00	11.22	N
ATOM	3674	N	ASP	C	153	60.175	27.014	50.719	1.00	12.72	N
ATOM	3675	CA	ASP	C	153	60.119	25.749	51.439	1.00	11.31	C
ATOM	3676	C	ASP	C	153	59.047	25.834	52.519	1.00	12.42	C
ATOM	3677	O	ASP	C	153	58.768	24.854	53.191	1.00	13.71	O
ATOM	3678	CB	ASP	C	153	61.462	25.409	52.096	1.00	9.61	C
ATOM	3679	CG	ASP	C	153	62.505	24.929	51.103	1.00	9.74	C
ATOM	3680	OD1	ASP	C	153	62.285	23.937	50.394	1.00	9.94	O
ATOM	3681	OD2	ASP	C	153	63.587	25.527	51.039	1.00	12.49	O
ATOM	3682	N	SER	C	154	58.438	27.001	52.693	1.00	14.62	N
ATOM	3683	CA	SER	C	154	57.407	27.158	53.712	1.00	15.40	C
ATOM	3684	C	SER	C	154	56.109	26.507	53.270	1.00	17.42	C
ATOM	3685	O	SER	C	154	55.578	26.816	52.206	1.00	18.74	O
ATOM	3686	CB	SER	C	154	57.183	28.639	54.034	1.00	14.80	C
ATOM	3687	OG	SER	C	154	56.473	28.813	55.254	1.00	10.64	O
ATOM	3688	N	GLY	C	155	55.599	25.612	54.105	1.00	18.91	N
ATOM	3689	CA	GLY	C	155	54.367	24.920	53.794	1.00	19.59	C
ATOM	3690	C	GLY	C	155	54.402	23.508	54.352	1.00	21.01	C
ATOM	3691	O	GLY	C	155	55.160	23.211	55.279	1.00	19.93	O
ATOM	3692	N	THR	C	156	53.612	22.621	53.758	1.00	21.99	N
ATOM	3693	CA	THR	C	156	53.550	21.241	54.209	1.00	22.98	C
ATOM	3694	C	THR	C	156	54.474	20.346	53.402	1.00	22.60	C
ATOM	3695	O	THR	C	156	54.344	20.257	52.180	1.00	25.02	O
ATOM	3696	CB	THR	C	156	52.125	20.678	54.086	1.00	24.04	C
ATOM	3697	OG1	THR	C	156	51.235	21.385	54.958	1.00	25.86	O
ATOM	3698	CG2	THR	C	156	52.111	19.219	54.432	1.00	25.42	C
ATOM	3699	N	TRP	C	157	55.421	19.713	54.086	1.00	21.34	N
ATOM	3700	CA	TRP	C	157	56.359	18.781	53.463	1.00	19.59	C
ATOM	3701	C	TRP	C	157	55.717	17.395	53.513	1.00	20.25	C
ATOM	3702	O	TRP	C	157	54.974	17.092	54.450	1.00	20.58	O
ATOM	3703	CB	TRP	C	157	57.679	18.753	54.234	1.00	15.84	C
ATOM	3704	CG	TRP	C	157	58.513	19.987	54.077	1.00	11.16	C
ATOM	3705	CD1	TRP	C	157	58.089	21.282	54.161	1.00	11.79	C
ATOM	3706	CD2	TRP	C	157	59.911	20.041	53.762	1.00	8.24	C
ATOM	3707	NE1	TRP	C	157	59.132	22.138	53.907	1.00	9.41	N
ATOM	3708	CE2	TRP	C	157	60.263	21.405	53.657	1.00	8.97	C
ATOM	3709	CE3	TRP	C	157	60.900	19.068	53.558	1.00	6.12	C
ATOM	3710	CZ2	TRP	C	157	61.564	21.826	53.353	1.00	9.57	C
ATOM	3711	CZ3	TRP	C	157	62.192	19.482	53.256	1.00	8.10	C
ATOM	3712	CH2	TRP	C	157	62.513	20.852	53.156	1.00	10.47	C
ATOM	3713	N	THR	C	158	55.976	16.569	52.501	1.00	21.03	N
ATOM	3714	CA	THR	C	158	55.418	15.218	52.449	1.00	20.80	C
ATOM	3715	C	THR	C	158	56.536	14.184	52.517	1.00	23.21	C
ATOM	3716	O	THR	C	158	57.338	14.054	51.587	1.00	22.06	O
ATOM	3717	CB	THR	C	158	54.606	14.992	51.172	1.00	18.83	C
ATOM	3718	OG1	THR	C	158	53.711	16.090	50.970	1.00	17.97	O
ATOM	3719	CG2	THR	C	158	53.799	13.708	51.280	1.00	17.76	C
ATOM	3720	N	CYS	C	159	56.562	13.441	53.617	1.00	26.27	N
ATOM	3721	CA	CYS	C	159	57.575	12.421	53.849	1.00	29.55	C
ATOM	3722	C	CYS	C	159	57.010	11.001	53.820	1.00	30.89	C
ATOM	3723	O	CYS	C	159	56.319	10.581	54.759	1.00	31.67	O
ATOM	3724	CB	CYS	C	159	58.260	12.685	55.188	1.00	30.96	C
ATOM	3725	SG	CYS	C	159	59.078	14.313	55.287	1.00	34.94	S

FIG. 53-61

ATOM	3727	CA	THR	C	160	56.825	8.898	52.558	1.00	29.44	C
ATOM	3728	C	THR	C	160	57.966	7.919	52.837	1.00	28.24	C
ATOM	3729	O	THR	C	160	59.019	7.976	52.191	1.00	27.56	O
ATOM	3730	CB	THR	C	160	56.264	8.651	51.130	1.00	30.04	C
ATOM	3731	OG1	THR	C	160	54.997	9.313	50.977	1.00	30.53	O
ATOM	3732	CG2	THR	C	160	56.086	7.167	50.873	1.00	29.78	C
ATOM	3733	N	VAL	C	161	57.763	7.057	53.830	1.00	27.85	N
ATOM	3734	CA	VAL	C	161	58.759	6.056	54.216	1.00	26.29	C
ATOM	3735	C	VAL	C	161	58.402	4.704	53.592	1.00	26.35	C
ATOM	3736	O	VAL	C	161	57.224	4.389	53.402	1.00	25.45	O
ATOM	3737	CB	VAL	C	161	58.849	5.921	55.752	1.00	24.73	C
ATOM	3738	CG1	VAL	C	161	59.797	4.811	56.139	1.00	23.11	C
ATOM	3739	CG2	VAL	C	161	59.325	7.217	56.351	1.00	23.75	C
ATOM	3740	N	LEU	C	162	59.416	3.905	53.288	1.00	25.96	N
ATOM	3741	CA	LEU	C	162	59.188	2.616	52.669	1.00	26.82	C
ATOM	3742	C	LEU	C	162	59.946	1.535	53.421	1.00	26.47	C
ATOM	3743	O	LEU	C	162	61.175	1.589	53.544	1.00	26.00	O
ATOM	3744	CB	LEU	C	162	59.627	2.671	51.199	1.00	29.28	C
ATOM	3745	CG	LEU	C	162	59.135	1.642	50.166	1.00	30.56	C
ATOM	3746	CD1	LEU	C	162	59.208	2.259	48.782	1.00	31.27	C
ATOM	3747	CD2	LEU	C	162	59.943	0.355	50.228	1.00	30.37	C
ATOM	3748	N	GLN	C	163	59.190	0.584	53.961	1.00	26.98	N
ATOM	3749	CA	GLN	C	163	59.721	-0.556	54.711	1.00	26.71	C
ATOM	3750	C	GLN	C	163	58.865	-1.754	54.317	1.00	27.66	C
ATOM	3751	O	GLN	C	163	57.635	-1.667	54.317	1.00	27.62	O
ATOM	3752	CB	GLN	C	163	59.608	-0.315	56.219	1.00	24.98	C
ATOM	3753	CG	GLN	C	163	59.890	-1.540	57.091	1.00	25.25	C
ATOM	3754	CD	GLN	C	163	61.352	-1.980	57.082	1.00	27.07	C
ATOM	3755	OE1	GLN	C	163	62.263	-1.161	56.930	1.00	26.36	O
ATOM	3756	NE2	GLN	C	163	61.583	-3.273	57.276	1.00	27.43	N
ATOM	3757	N	ASN	C	164	59.517	-2.852	53.936	1.00	28.18	N
ATOM	3758	CA	ASN	C	164	58.820	-4.074	53.524	1.00	27.28	C
ATOM	3759	C	ASN	C	164	57.828	-3.806	52.400	1.00	28.24	C
ATOM	3760	O	ASN	C	164	56.665	-4.187	52.499	1.00	27.33	O
ATOM	3761	CB	ASN	C	164	58.061	-4.715	54.697	1.00	25.86	C
ATOM	3762	CG	ASN	C	164	58.962	-5.104	55.844	1.00	23.54	C
ATOM	3763	OD1	ASN	C	164	59.178	-4.324	56.761	1.00	24.92	O
ATOM	3764	ND2	ASN	C	164	59.484	-6.315	55.805	1.00	22.09	N
ATOM	3765	N	GLN	C	165	58.273	-3.108	51.356	1.00	30.69	N
ATOM	3766	CA	GLN	C	165	57.422	-2.815	50.204	1.00	33.45	C
ATOM	3767	C	GLN	C	165	56.179	-2.018	50.597	1.00	34.13	C
ATOM	3768	O	GLN	C	165	55.264	-1.836	49.785	1.00	33.27	O
ATOM	3769	CB	GLN	C	165	57.021	-4.141	49.546	1.00	38.26	C
ATOM	3770	CG	GLN	C	165	56.205	-4.055	48.273	1.00	43.02	C
ATOM	3771	CD	GLN	C	165	55.592	-5.399	47.917	1.00	44.68	C
ATOM	3772	OE1	GLN	C	165	56.250	-6.261	47.335	1.00	45.21	O
ATOM	3773	NE2	GLN	C	165	54.342	-5.600	48.311	1.00	45.67	N
ATOM	3774	N	LYS	C	166	56.159	-1.535	51.839	1.00	35.23	N
ATOM	3775	CA	LYS	C	166	55.040	-0.759	52.371	1.00	35.64	C
ATOM	3776	C	LYS	C	166	55.434	0.697	52.575	1.00	36.20	C
ATOM	3777	O	LYS	C	166	56.621	1.010	52.717	1.00	36.47	O
ATOM	3778	CB	LYS	C	166	54.550	-1.356	53.694	1.00	34.32	C
ATOM	3779	CG	LYS	C	166	53.805	-2.670	53.544	1.00	31.93	C
ATOM	3780	CD	LYS	C	166	52.726	-2.536	52.490	1.00	32.10	C
ATOM	3781	CE	LYS	C	166	51.630	-3.542	52.697	1.00	32.61	C
ATOM	3782	NZ	LYS	C	166	51.076	-3.407	54.073	1.00	35.68	N
ATOM	3783	N	LYS	C	167	54.438	1.582	52.609	1.00	36.33	N
ATOM	3784	CA	LYS	C	167	54.707	3.004	52.776	1.00	35.96	C
ATOM	3785	C	LYS	C	167	53.693	3.782	53.608	1.00	34.21	C
ATOM	3786	O	LYS	C	167	52.486	3.622	53.453	1.00	33.28	O
ATOM	3787	CB	LYS	C	167	54.836	3.690	51.406	1.00	37.91	C
ATOM	3788	CG	LYS	C	167	53.526	3.825	50.623	1.00	41.44	C
ATOM	3789	CD	LYS	C	167	53.272	5.269	50.161	1.00	45.13	C
ATOM	3790	CE	LYS	C	167	52.757	6.171	51.290	1.00	46.91	C
ATOM	3791	NZ	LYS	C	167	52.666	7.622	50.894	1.00	50.08	N
ATOM	3792	N	VAL	C	168	54.207	4.634	54.485	1.00	33.66	N
ATOM	3793	CA	VAL	C	168	53.387	5.508	55.313	1.00	32.71	C
ATOM	3794	C	VAL	C	168	53.762	6.918	54.874	1.00	31.76	C
ATOM	3795	O	VAL	C	168	54.911	7.167	54.477	1.00	30.63	O
ATOM	3796	CB	VAL	C	168	53.643	5.334	56.833	1.00	32.93	C

FIG. 53-62

ATOM	3798	CG2	VAL	C	168	55.129	5.220	57.129	1.00	32.67	C
ATOM	3799	N	GLU	C	169	52.779	7.815	54.892	1.00	31.71	N
ATOM	3800	CA	GLU	C	169	52.967	9.204	54.469	1.00	30.89	C
ATOM	3801	C	GLU	C	169	52.908	10.141	55.670	1.00	29.82	C
ATOM	3802	O	GLU	C	169	51.959	10.078	56.463	1.00	29.23	O
ATOM	3803	CB	GLU	C	169	51.883	9.560	53.454	1.00	31.18	C
ATOM	3804	CG	GLU	C	169	52.069	10.876	52.745	1.00	32.95	C
ATOM	3805	CD	GLU	C	169	51.017	11.105	51.684	1.00	32.44	C
ATOM	3806	OE1	GLU	C	169	50.987	10.316	50.716	1.00	36.25	O
ATOM	3807	OE2	GLU	C	169	50.219	12.056	51.821	1.00	31.12	O
ATOM	3808	N	PHE	C	170	53.917	11.001	55.790	1.00	28.79	N
ATOM	3809	CA	PHE	C	170	54.026	11.952	56.899	1.00	28.29	C
ATOM	3810	C	PHE	C	170	54.136	13.396	56.407	1.00	27.47	C
ATOM	3811	O	PHE	C	170	55.215	13.836	56.008	1.00	27.61	O
ATOM	3812	CB	PHE	C	170	55.281	11.661	57.739	1.00	29.48	C
ATOM	3813	CG	PHE	C	170	55.233	10.382	58.518	1.00	29.76	C
ATOM	3814	CD1	PHE	C	170	54.314	10.206	59.550	1.00	30.83	C
ATOM	3815	CD2	PHE	C	170	56.146	9.365	58.257	1.00	30.55	C
ATOM	3816	CE1	PHE	C	170	54.316	9.038	60.318	1.00	30.05	C
ATOM	3817	CE2	PHE	C	170	56.155	8.193	59.020	1.00	30.30	C
ATOM	3818	CZ	PHE	C	170	55.236	8.030	60.050	1.00	29.19	C
ATOM	3819	N	LYS	C	171	53.042	14.145	56.454	1.00	26.50	N
ATOM	3820	CA	LYS	C	171	53.068	15.541	56.026	1.00	25.38	C
ATOM	3821	C	LYS	C	171	53.494	16.403	57.213	1.00	24.25	C
ATOM	3822	O	LYS	C	171	52.856	16.347	58.260	1.00	25.65	O
ATOM	3823	CB	LYS	C	171	51.682	15.954	55.542	1.00	25.88	C
ATOM	3824	CG	LYS	C	171	51.206	15.200	54.314	1.00	25.96	C
ATOM	3825	CD	LYS	C	171	49.782	15.602	53.942	1.00	28.50	C
ATOM	3826	CE	LYS	C	171	49.730	17.011	53.362	1.00	29.70	C
ATOM	3827	NZ	LYS	C	171	48.342	17.504	53.122	1.00	29.71	N
ATOM	3828	N	ILE	C	172	54.574	17.172	57.071	1.00	22.36	N
ATOM	3829	CA	ILE	C	172	55.082	18.024	58.162	1.00	20.16	C
ATOM	3830	C	ILE	C	172	55.199	19.493	57.737	1.00	19.90	C
ATOM	3831	O	ILE	C	172	55.846	19.803	56.745	1.00	19.88	O
ATOM	3832	CB	ILE	C	172	56.491	17.573	58.627	1.00	19.36	C
ATOM	3833	CG1	ILE	C	172	56.653	16.043	58.542	1.00	18.58	C
ATOM	3834	CG2	ILE	C	172	56.745	18.058	60.046	1.00	19.32	C
ATOM	3835	CD1	ILE	C	172	56.013	15.247	59.677	1.00	17.14	C
ATOM	3836	N	ASP	C	173	54.640	20.397	58.535	1.00	20.38	N
ATOM	3837	CA	ASP	C	173	54.649	21.829	58.230	1.00	19.82	C
ATOM	3838	C	ASP	C	173	55.888	22.566	58.698	1.00	19.67	C
ATOM	3839	O	ASP	C	173	56.191	22.585	59.888	1.00	19.89	O
ATOM	3840	CB	ASP	C	173	53.418	22.513	58.843	1.00	20.41	C
ATOM	3841	CG	ASP	C	173	52.123	22.073	58.202	1.00	20.60	C
ATOM	3842	OD1	ASP	C	173	51.725	20.902	58.381	1.00	22.57	O
ATOM	3843	OD2	ASP	C	173	51.496	22.894	57.513	1.00	21.31	O
ATOM	3844	N	ILE	C	174	56.582	23.203	57.764	1.00	19.91	N
ATOM	3845	CA	ILE	C	174	57.778	23.981	58.075	1.00	19.69	C
ATOM	3846	C	ILE	C	174	57.437	25.432	57.737	1.00	18.43	C
ATOM	3847	O	ILE	C	174	56.721	25.686	56.762	1.00	17.50	O
ATOM	3848	CB	ILE	C	174	58.995	23.580	57.181	1.00	21.54	C
ATOM	3849	CG1	ILE	C	174	59.186	22.061	57.138	1.00	23.72	C
ATOM	3850	CG2	ILE	C	174	60.265	24.227	57.708	1.00	22.56	C
ATOM	3851	CD1	ILE	C	174	59.535	21.423	58.473	1.00	24.97	C
ATOM	3852	N	VAL	C	175	57.927	26.379	58.530	1.00	15.80	N
ATOM	3853	CA	VAL	C	175	57.672	27.784	58.248	1.00	15.23	C
ATOM	3854	C	VAL	C	175	58.984	28.538	58.046	1.00	15.59	C
ATOM	3855	O	VAL	C	175	59.722	28.783	58.999	1.00	14.83	O
ATOM	3856	CB	VAL	C	175	56.848	28.479	59.367	1.00	15.13	C
ATOM	3857	CG1	VAL	C	175	56.780	29.991	59.118	1.00	11.47	C
ATOM	3858	CG2	VAL	C	175	55.447	27.891	59.438	1.00	13.88	C
ATOM	3859	N	VAL	C	176	59.285	28.885	56.802	1.00	15.76	N
ATOM	3860	CA	VAL	C	176	60.498	29.637	56.508	1.00	16.89	C
ATOM	3861	C	VAL	C	176	60.088	31.109	56.400	1.00	18.51	C
ATOM	3862	O	VAL	C	176	59.476	31.537	55.411	1.00	19.47	O
ATOM	3863	CB	VAL	C	176	61.148	29.174	55.202	1.00	17.23	C
ATOM	3864	CG1	VAL	C	176	62.568	29.713	55.115	1.00	18.51	C
ATOM	3865	CG2	VAL	C	176	61.133	27.653	55.123	1.00	16.01	C
ATOM	3866	N	LEU	C	177	60.374	31.855	57.462	1.00	18.16	N
ATOM	3867	CA	LEU	C	177	60.047	33.269	57.577	1.00	17.22	C

FIG. 53-63

ATOM	3869	O	LEU	C	177	61.678	33.966	55.944	1.00	17.36	O
ATOM	3870	CB	LEU	C	177	60.575	33.798	58.906	1.00	16.95	C
ATOM	3871	CG	LEU	C	177	59.568	34.354	59.908	1.00	15.24	C
ATOM	3872	CD1	LEU	C	177	58.294	33.532	59.933	1.00	16.51	C
ATOM	3873	CD2	LEU	C	177	60.212	34.369	61.270	1.00	18.02	C
ATOM	3874	N	ALA	C	178	59.722	35.099	56.046	1.00	17.39	N
ATOM	3875	CA	ALA	C	178	60.050	36.037	54.981	1.00	18.66	C
ATOM	3876	C	ALA	C	178	60.698	37.296	55.555	1.00	19.74	C
ATOM	3877	O	ALA	C	178	60.512	37.617	56.731	1.00	19.40	O
ATOM	3878	CB	ALA	C	178	58.805	36.389	54.197	1.00	17.39	C
ATOM	3879	N	PHE	C	179	61.449	38.007	54.719	1.00	22.31	N
ATOM	3880	CA	PHE	C	179	62.136	39.225	55.142	1.00	25.40	C
ATOM	3881	C	PHE	C	179	62.398	40.152	53.959	1.00	29.04	C
ATOM	3882	O	PHE	C	179	62.740	39.698	52.859	1.00	30.27	O
ATOM	3883	CB	PHE	C	179	63.468	38.885	55.803	1.00	23.89	C
ATOM	3884	CG	PHE	C	179	64.529	38.418	54.842	1.00	23.56	C
ATOM	3885	CD1	PHE	C	179	64.566	37.103	54.407	1.00	24.11	C
ATOM	3886	CD2	PHE	C	179	65.516	39.292	54.403	1.00	23.56	C
ATOM	3887	CE1	PHE	C	179	65.574	36.661	53.555	1.00	25.53	C
ATOM	3888	CE2	PHE	C	179	66.528	38.857	53.550	1.00	25.32	C
ATOM	3889	CZ	PHE	C	179	66.558	37.541	53.127	1.00	24.42	C
ATOM	3890	N	GLN	C	180	62.252	41.451	54.188	1.00	31.01	N
ATOM	3891	CA	GLN	C	180	62.485	42.428	53.136	1.00	31.97	C
ATOM	3892	C	GLN	C	180	63.836	43.125	53.282	1.00	32.39	C
ATOM	3893	O	GLN	C	180	64.428	43.146	54.366	1.00	33.39	O
ATOM	3894	CB	GLN	C	180	61.353	43.454	53.094	1.00	32.09	C
ATOM	3895	CG	GLN	C	180	60.438	43.300	51.897	1.00	33.19	C
ATOM	3896	CD	GLN	C	180	61.176	43.467	50.582	1.00	33.40	C
ATOM	3897	OE1	GLN	C	180	62.101	42.717	50.276	1.00	34.04	O
ATOM	3898	NE2	GLN	C	180	60.764	44.445	49.793	1.00	34.51	N
ATOM	3899	N	LYS	C	181	64.329	43.661	52.171	1.00	32.34	N
ATOM	3900	CA	LYS	C	181	65.603	44.362	52.134	1.00	31.99	C
ATOM	3901	C	LYS	C	181	65.577	45.584	53.038	1.00	32.66	C
ATOM	3902	O	LYS	C	181	64.692	46.432	52.800	1.00	33.70	O
ATOM	3903	CB	LYS	C	181	65.924	44.794	50.698	1.00	31.91	C
ATOM	3904	CG	LYS	C	181	66.260	43.655	49.748	1.00	31.31	C
ATOM	3905	CD	LYS	C	181	67.506	42.908	50.200	1.00	32.09	C
ATOM	3906	CE	LYS	C	181	68.738	43.806	50.183	1.00	33.37	C
ATOM	3907	NZ	LYS	C	181	69.879	43.175	50.893	1.00	33.00	N
TER	3908		LYS	C	181						
ATOM	3909	N	GLU	L	1	-0.316	8.025	77.827	1.00	31.44	N
ATOM	3910	CA	GLU	L	1	-1.773	8.334	77.694	1.00	32.29	C
ATOM	3911	C	GLU	L	1	-2.361	8.914	78.981	1.00	30.69	C
ATOM	3912	O	GLU	L	1	-3.575	8.928	79.169	1.00	30.35	O
ATOM	3913	CB	GLU	L	1	-2.545	7.081	77.275	1.00	34.07	C
ATOM	3914	CG	GLU	L	1	-3.795	7.366	76.458	1.00	36.70	C
ATOM	3915	CD	GLU	L	1	-4.126	6.250	75.473	1.00	40.14	C
ATOM	3916	OE1	GLU	L	1	-3.560	5.138	75.605	1.00	39.72	O
ATOM	3917	OE2	GLU	L	1	-4.946	6.489	74.554	1.00	41.19	O
ATOM	3918	N	LEU	L	2	-1.492	9.391	79.867	1.00	29.92	N
ATOM	3919	CA	LEU	L	2	-1.922	9.995	81.128	1.00	28.31	C
ATOM	3920	C	LEU	L	2	-2.433	11.410	80.874	1.00	28.41	C
ATOM	3921	O	LEU	L	2	-1.743	12.223	80.250	1.00	27.72	O
ATOM	3922	CB	LEU	L	2	-0.754	10.058	82.115	1.00	25.05	C
ATOM	3923	CG	LEU	L	2	-0.670	9.013	83.225	1.00	23.51	C
ATOM	3924	CD1	LEU	L	2	-1.767	9.288	84.218	1.00	24.46	C
ATOM	3925	CD2	LEU	L	2	-0.759	7.600	82.677	1.00	18.26	C
ATOM	3926	N	GLU	L	3	-3.664	11.675	81.297	1.00	28.26	N
ATOM	3927	CA	GLU	L	3	-4.249	12.996	81.129	1.00	27.49	C
ATOM	3928	C	GLU	L	3	-4.207	13.689	82.485	1.00	26.05	C
ATOM	3929	O	GLU	L	3	-4.782	13.202	83.467	1.00	26.90	O
ATOM	3930	CB	GLU	L	3	-5.679	12.888	80.606	1.00	28.46	C
ATOM	3931	CG	GLU	L	3	-6.274	14.211	80.162	1.00	33.07	C
ATOM	3932	CD	GLU	L	3	-7.317	14.733	81.128	1.00	36.39	C
ATOM	3933	OE1	GLU	L	3	-6.982	14.931	82.314	1.00	38.96	O
ATOM	3934	OE2	GLU	L	3	-8.475	14.932	80.703	1.00	36.94	O
ATOM	3935	N	LEU	L	4	-3.466	14.788	82.543	1.00	23.66	N
ATOM	3936	CA	LEU	L	4	-3.300	15.558	83.768	1.00	20.72	C
ATOM	3937	C	LEU	L	4	-4.177	16.809	83.771	1.00	20.47	C
ATOM	3938	O	LEU	L	4	-4.431	17.412	82.722	1.00	19.71	O

FIG. 53-64

ATOM	3940	CG	LEU	L	4	-0.903	14.698	84.119	1.00	15.50	C
ATOM	3941	CD1	LEU	L	4	0.535	15.079	83.893	1.00	15.51	C
ATOM	3942	CD2	LEU	L	4	-1.073	14.113	85.500	1.00	14.36	C
ATOM	3943	N	THR	L	5	-4.646	17.194	84.955	1.00	19.86	N
ATOM	3944	CA	THR	L	5	-5.516	18.357	85.093	1.00	19.04	C
ATOM	3945	C	THR	L	5	-5.189	19.082	86.373	1.00	19.42	C
ATOM	3946	O	THR	L	5	-5.033	18.458	87.420	1.00	21.99	O
ATOM	3947	CB	THR	L	5	-7.010	17.958	85.197	1.00	18.26	C
ATOM	3948	OG1	THR	L	5	-7.406	17.182	84.057	1.00	16.67	O
ATOM	3949	CG2	THR	L	5	-7.878	19.197	85.299	1.00	16.92	C
ATOM	3950	N	GLN	L	6	-5.085	20.401	86.287	1.00	18.59	N
ATOM	3951	CA	GLN	L	6	-4.814	21.221	87.451	1.00	17.69	C
ATOM	3952	C	GLN	L	6	-6.155	21.905	87.682	1.00	20.76	C
ATOM	3953	O	GLN	L	6	-6.705	22.543	86.779	1.00	19.35	O
ATOM	3954	CB	GLN	L	6	-3.667	22.175	87.146	1.00	14.41	C
ATOM	3955	CG	GLN	L	6	-2.452	21.397	86.637	1.00	10.06	C
ATOM	3956	CD	GLN	L	6	-1.225	22.237	86.407	1.00	7.80	C
ATOM	3957	OE1	GLN	L	6	-0.471	22.015	85.457	1.00	6.57	O
ATOM	3958	NE2	GLN	L	6	-1.007	23.201	87.272	1.00	8.61	N
ATOM	3959	N	SER	L	7	-6.724	21.644	88.857	1.00	25.00	N
ATOM	3960	CA	SER	L	7	-8.047	22.132	89.245	1.00	27.51	C
ATOM	3961	C	SER	L	7	-8.334	23.626	89.169	1.00	27.97	C
ATOM	3962	O	SER	L	7	-9.099	24.063	88.300	1.00	30.44	O
ATOM	3963	CB	SER	L	7	-8.440	21.547	90.600	1.00	29.38	C
ATOM	3964	OG	SER	L	7	-8.318	20.128	90.588	1.00	32.11	O
ATOM	3965	N	PRO	L	8	-7.754	24.438	90.070	1.00	26.22	N
ATOM	3966	CA	PRO	L	8	-8.063	25.872	89.949	1.00	24.93	C
ATOM	3967	C	PRO	L	8	-7.308	26.492	88.758	1.00	24.76	C
ATOM	3968	O	PRO	L	8	-6.081	26.631	88.790	1.00	24.81	O
ATOM	3969	CB	PRO	L	8	-7.589	26.428	91.290	1.00	24.11	C
ATOM	3970	CG	PRO	L	8	-6.386	25.576	91.590	1.00	24.77	C
ATOM	3971	CD	PRO	L	8	-6.817	24.181	91.180	1.00	24.26	C
ATOM	3972	N	ALA	L	9	-8.033	26.814	87.690	1.00	23.55	N
ATOM	3973	CA	ALA	L	9	-7.415	27.403	86.502	1.00	21.35	C
ATOM	3974	C	ALA	L	9	-6.713	28.709	86.844	1.00	20.25	C
ATOM	3975	O	ALA	L	9	-5.674	29.042	86.256	1.00	20.22	O
ATOM	3976	CB	ALA	L	9	-8.454	27.630	85.422	1.00	21.24	C
ATOM	3977	N	THR	L	10	-7.298	29.453	87.779	1.00	19.33	N
ATOM	3978	CA	THR	L	10	-6.742	30.724	88.231	1.00	18.37	C
ATOM	3979	C	THR	L	10	-6.945	30.852	89.744	1.00	17.83	C
ATOM	3980	O	THR	L	10	-8.058	30.663	90.255	1.00	17.66	O
ATOM	3981	CB	THR	L	10	-7.411	31.932	87.524	1.00	19.55	C
ATOM	3982	OG1	THR	L	10	-8.177	31.484	86.393	1.00	21.65	O
ATOM	3983	CG2	THR	L	10	-6.356	32.913	87.050	1.00	17.75	C
ATOM	3984	N	LEU	L	11	-5.861	31.118	90.464	1.00	16.23	N
ATOM	3985	CA	LEU	L	11	-5.933	31.276	91.907	1.00	15.32	C
ATOM	3986	C	LEU	L	11	-5.573	32.720	92.270	1.00	15.02	C
ATOM	3987	O	LEU	L	11	-4.500	33.219	91.901	1.00	12.98	O
ATOM	3988	CB	LEU	L	11	-4.980	30.308	92.613	1.00	14.18	C
ATOM	3989	CG	LEU	L	11	-5.226	30.185	94.115	1.00	13.89	C
ATOM	3990	CD1	LEU	L	11	-6.534	29.461	94.361	1.00	14.46	C
ATOM	3991	CD2	LEU	L	11	-4.086	29.440	94.758	1.00	14.10	C
ATOM	3992	N	SER	L	12	-6.479	33.382	92.986	1.00	15.52	N
ATOM	3993	CA	SER	L	12	-6.291	34.766	93.398	1.00	15.65	C
ATOM	3994	C	SER	L	12	-5.992	34.813	94.893	1.00	16.19	C
ATOM	3995	O	SER	L	12	-6.873	34.550	95.718	1.00	17.01	O
ATOM	3996	CB	SER	L	12	-7.559	35.573	93.083	1.00	16.63	C
ATOM	3997	OG	SER	L	12	-7.962	35.433	91.719	1.00	16.33	O
ATOM	3998	N	VAL	L	13	-4.758	35.162	95.243	1.00	15.69	N
ATOM	3999	CA	VAL	L	13	-4.337	35.232	96.642	1.00	15.92	C
ATOM	4000	C	VAL	L	13	-3.636	36.547	97.008	1.00	15.53	C
ATOM	4001	O	VAL	L	13	-2.892	37.112	96.207	1.00	14.64	O
ATOM	4002	CB	VAL	L	13	-3.389	34.059	97.000	1.00	16.50	C
ATOM	4003	CG1	VAL	L	13	-4.162	32.750	97.068	1.00	17.04	C
ATOM	4004	CG2	VAL	L	13	-2.282	33.949	95.961	1.00	17.84	C
ATOM	4005	N	SER	L	14	-3.881	37.029	98.222	1.00	15.24	N
ATOM	4006	CA	SER	L	14	-3.265	38.258	98.702	1.00	16.02	C
ATOM	4007	C	SER	L	14	-1.807	37.949	99.074	1.00	15.89	C
ATOM	4008	O	SER	L	14	-1.534	36.976	99.779	1.00	17.69	O
ATOM	4009	CB	SER	L	14	-4.041	38.704	99.907	1.00	17.34	C

FIG. 53-65

ATOM	4011	N	PRO	L	15	-0.860	38.810	98.662	1.00	14.23	N
ATOM	4012	CA	PRO	L	15	0.562	38.602	98.952	1.00	13.05	C
ATOM	4013	C	PRO	L	15	0.814	38.343	100.423	1.00	13.44	C
ATOM	4014	O	PRO	L	15	0.259	39.025	101.281	1.00	16.17	O
ATOM	4015	CB	PRO	L	15	1.196	39.934	98.548	1.00	12.79	C
ATOM	4016	CG	PRO	L	15	0.226	40.529	97.590	1.00	13.35	C
ATOM	4017	CD	PRO	L	15	-1.095	40.185	98.191	1.00	13.28	C
ATOM	4018	N	GLY	L	16	1.672	37.378	100.711	1.00	12.99	N
ATOM	4019	CA	GLY	L	16	2.005	37.070	102.085	1.00	12.12	C
ATOM	4020	C	GLY	L	16	1.178	35.955	102.674	1.00	13.08	C
ATOM	4021	O	GLY	L	16	1.571	35.374	103.684	1.00	13.68	O
ATOM	4022	N	GLU	L	17	0.009	35.706	102.092	1.00	14.80	N
ATOM	4023	CA	GLU	L	17	-0.897	34.639	102.533	1.00	15.89	C
ATOM	4024	C	GLU	L	17	-0.392	33.287	102.009	1.00	15.65	C
ATOM	4025	O	GLU	L	17	0.686	33.215	101.432	1.00	15.62	O
ATOM	4026	CB	GLU	L	17	-2.300	34.899	101.975	1.00	16.44	C
ATOM	4027	CG	GLU	L	17	-3.380	35.066	103.022	1.00	20.28	C
ATOM	4028	CD	GLU	L	17	-3.811	36.507	103.218	1.00	23.46	C
ATOM	4029	OE1	GLU	L	17	-3.203	37.410	102.601	1.00	26.76	O
ATOM	4030	OE2	GLU	L	17	-4.768	36.747	103.993	1.00	23.58	O
ATOM	4031	N	ARG	L	18	-1.199	32.241	102.162	1.00	17.45	N
ATOM	4032	CA	ARG	L	18	-0.856	30.892	101.709	1.00	18.54	C
ATOM	4033	C	ARG	L	18	-1.681	30.440	100.496	1.00	19.46	C
ATOM	4034	O	ARG	L	18	-2.878	30.738	100.409	1.00	21.63	O
ATOM	4035	CB	ARG	L	18	-1.064	29.910	102.857	1.00	19.38	C
ATOM	4036	CG	ARG	L	18	-1.083	28.442	102.460	1.00	20.71	C
ATOM	4037	CD	ARG	L	18	-1.373	27.569	103.660	1.00	20.07	C
ATOM	4038	NE	ARG	L	18	-0.260	27.536	104.602	1.00	22.13	N
ATOM	4039	CZ	ARG	L	18	0.415	26.431	104.907	1.00	24.21	C
ATOM	4040	NH1	ARG	L	18	0.081	25.280	104.331	1.00	23.29	N
ATOM	4041	NH2	ARG	L	18	1.405	26.467	105.795	1.00	24.99	N
ATOM	4042	N	ALA	L	19	-1.049	29.683	99.595	1.00	18.65	N
ATOM	4043	CA	ALA	L	19	-1.702	29.155	98.378	1.00	16.57	C
ATOM	4044	C	ALA	L	19	-1.544	27.629	98.196	1.00	13.56	C
ATOM	4045	O	ALA	L	19	-0.500	27.060	98.496	1.00	11.67	O
ATOM	4046	CB	ALA	L	19	-1.173	29.883	97.145	1.00	14.46	C
ATOM	4047	N	THR	L	20	-2.584	26.980	97.688	1.00	12.77	N
ATOM	4048	CA	THR	L	20	-2.573	25.535	97.463	1.00	12.50	C
ATOM	4049	C	THR	L	20	-3.238	25.158	96.137	1.00	11.49	C
ATOM	4050	O	THR	L	20	-4.430	25.411	95.946	1.00	11.49	O
ATOM	4051	CB	THR	L	20	-3.259	24.789	98.646	1.00	12.82	C
ATOM	4052	OG1	THR	L	20	-2.272	24.409	99.619	1.00	12.71	O
ATOM	4053	CG2	THR	L	20	-4.023	23.559	98.164	1.00	13.86	C
ATOM	4054	N	LEU	L	21	-2.471	24.522	95.250	1.00	11.90	N
ATOM	4055	CA	LEU	L	21	-2.952	24.106	93.923	1.00	13.41	C
ATOM	4056	C	LEU	L	21	-3.006	22.580	93.754	1.00	15.85	C
ATOM	4057	O	LEU	L	21	-2.062	21.877	94.114	1.00	16.34	O
ATOM	4058	CB	LEU	L	21	-2.038	24.673	92.838	1.00	10.60	C
ATOM	4059	CG	LEU	L	21	-1.291	25.990	93.057	1.00	9.16	C
ATOM	4060	CD1	LEU	L	21	-0.495	26.310	91.801	1.00	7.83	C
ATOM	4061	CD2	LEU	L	21	-2.243	27.113	93.366	1.00	8.13	C
ATOM	4062	N	SER	L	22	-4.072	22.079	93.134	1.00	17.86	N
ATOM	4063	CA	SER	L	22	-4.234	20.639	92.927	1.00	18.46	C
ATOM	4064	C	SER	L	22	-4.021	20.166	91.491	1.00	18.18	C
ATOM	4065	O	SER	L	22	-4.403	20.849	90.532	1.00	18.53	O
ATOM	4066	CB	SER	L	22	-5.611	20.184	93.423	1.00	20.56	C
ATOM	4067	OG	SER	L	22	-6.650	21.002	92.910	1.00	22.97	O
ATOM	4068	N	CYS	L	23	-3.460	18.967	91.356	1.00	17.73	N
ATOM	4069	CA	CYS	L	23	-3.176	18.355	90.059	1.00	17.22	C
ATOM	4070	C	CYS	L	23	-3.592	16.886	90.057	1.00	18.28	C
ATOM	4071	O	CYS	L	23	-2.934	16.042	90.680	1.00	19.49	O
ATOM	4072	CB	CYS	L	23	-1.685	18.459	89.760	1.00	16.10	C
ATOM	4073	SG	CYS	L	23	-1.058	17.315	88.491	1.00	15.24	S
ATOM	4074	N	ARG	L	24	-4.701	16.589	89.390	1.00	17.66	N
ATOM	4075	CA	ARG	L	24	-5.201	15.227	89.308	1.00	19.01	C
ATOM	4076	C	ARG	L	24	-4.729	14.531	88.026	1.00	19.38	C
ATOM	4077	O	ARG	L	24	-4.286	15.191	87.079	1.00	19.33	O
ATOM	4078	CB	ARG	L	24	-6.741	15.235	89.389	1.00	21.08	C
ATOM	4079	CG	ARG	L	24	-7.483	14.343	88.364	1.00	21.37	C
ATOM	4080	CD	ARG	L	24	-8.101	15.175	87.238	1.00	23.45	C

FIG. 53-66

ATOM	4082	CZ	ARG L	24	-8.028	13.949	85.105	1.00	21.21	C
ATOM	4083	NH1	ARG L	24	-6.747	14.265	84.949	1.00	18.73	N
ATOM	4084	NH2	ARG L	24	-8.646	13.226	84.177	1.00	21.96	N
ATOM	4085	N	ALA L	25	-4.842	13.202	88.008	1.00	19.40	N
ATOM	4086	CA	ALA L	25	-4.486	12.376	86.854	1.00	18.37	C
ATOM	4087	C	ALA L	25	-5.646	11.409	86.562	1.00	18.52	C
ATOM	4088	O	ALA L	25	-6.455	11.108	87.444	1.00	18.35	O
ATOM	4089	CB	ALA L	25	-3.209	11.608	87.127	1.00	15.31	C
ATOM	4090	N	SER L	26	-5.765	10.977	85.311	1.00	19.56	N
ATOM	4091	CA	SER L	26	-6.826	10.051	84.899	1.00	19.32	C
ATOM	4092	C	SER L	26	-6.446	8.609	85.202	1.00	20.08	C
ATOM	4093	O	SER L	26	-7.300	7.734	85.293	1.00	19.11	O
ATOM	4094	CB	SER L	26	-7.099	10.202	83.400	1.00	19.52	C
ATOM	4095	OG	SER L	26	-5.890	10.143	82.650	1.00	19.21	O
ATOM	4096	N	GLU L	27	-5.149	8.383	85.369	1.00	21.48	N
ATOM	4097	CA	GLU L	27	-4.606	7.062	85.651	1.00	22.68	C
ATOM	4098	C	GLU L	27	-3.615	7.299	86.784	1.00	21.55	C
ATOM	4099	O	GLU L	27	-3.297	8.449	87.075	1.00	20.70	O
ATOM	4100	CB	GLU L	27	-3.894	6.538	84.397	1.00	24.20	C
ATOM	4101	CG	GLU L	27	-3.422	5.100	84.464	1.00	26.70	C
ATOM	4102	CD	GLU L	27	-2.802	4.629	83.161	1.00	28.70	C
ATOM	4103	OE1	GLU L	27	-3.303	5.005	82.077	1.00	26.39	O
ATOM	4104	OE2	GLU L	27	-1.808	3.875	83.223	1.00	31.38	O
ATOM	4105	N	SER L	28	-3.131	6.239	87.430	1.00	20.23	N
ATOM	4106	CA	SER L	28	-2.190	6.431	88.526	1.00	18.82	C
ATOM	4107	C	SER L	28	-0.789	6.746	88.030	1.00	19.09	C
ATOM	4108	O	SER L	28	-0.262	6.066	87.145	1.00	17.76	O
ATOM	4109	CB	SER L	28	-2.153	5.229	89.460	1.00	18.00	C
ATOM	4110	OG	SER L	28	-1.426	5.543	90.645	1.00	14.69	O
ATOM	4111	N	VAL L	29	-0.199	7.768	88.650	1.00	18.80	N
ATOM	4112	CA	VAL L	29	1.135	8.266	88.334	1.00	17.92	C
ATOM	4113	C	VAL L	29	2.209	7.771	89.324	1.00	17.57	C
ATOM	4114	O	VAL L	29	3.407	7.919	89.092	1.00	15.94	O
ATOM	4115	CB	VAL L	29	1.094	9.814	88.277	1.00	18.83	C
ATOM	4116	CG1	VAL L	29	2.479	10.388	88.093	1.00	20.20	C
ATOM	4117	CG2	VAL L	29	0.178	10.268	87.154	1.00	16.01	C
ATOM	4118	N	SER L	30	1.757	7.238	90.451	1.00	19.43	N
ATOM	4119	CA	SER L	30	2.621	6.680	91.493	1.00	21.15	C
ATOM	4120	C	SER L	30	3.892	7.446	91.899	1.00	22.67	C
ATOM	4121	O	SER L	30	4.993	6.888	91.885	1.00	24.62	O
ATOM	4122	CB	SER L	30	2.963	5.228	91.136	1.00	21.43	C
ATOM	4123	OG	SER L	30	3.696	4.586	92.164	1.00	24.65	O
ATOM	4124	N	SER L	31	3.728	8.694	92.330	1.00	21.72	N
ATOM	4125	CA	SER L	31	4.843	9.535	92.787	1.00	21.00	C
ATOM	4126	C	SER L	31	5.684	10.211	91.715	1.00	20.70	C
ATOM	4127	O	SER L	31	6.423	11.155	92.020	1.00	20.56	O
ATOM	4128	CB	SER L	31	5.766	8.798	93.773	1.00	20.26	C
ATOM	4129	OG	SER L	31	5.092	8.474	94.979	1.00	17.50	O
ATOM	4130	N	ASP L	32	5.569	9.756	90.471	1.00	18.99	N
ATOM	4131	CA	ASP L	32	6.321	10.372	89.383	1.00	16.73	C
ATOM	4132	C	ASP L	32	5.619	11.645	88.924	1.00	15.84	C
ATOM	4133	O	ASP L	32	5.078	11.708	87.820	1.00	16.03	O
ATOM	4134	CB	ASP L	32	6.493	9.389	88.228	1.00	15.22	C
ATOM	4135	CG	ASP L	32	7.479	8.293	88.548	1.00	14.08	C
ATOM	4136	OD1	ASP L	32	8.686	8.593	88.640	1.00	14.00	O
ATOM	4137	OD2	ASP L	32	7.052	7.134	88.732	1.00	14.42	O
ATOM	4138	N	LEU L	33	5.616	12.651	89.797	1.00	16.26	N
ATOM	4139	CA	LEU L	33	4.978	13.942	89.524	1.00	14.57	C
ATOM	4140	C	LEU L	33	5.983	15.063	89.770	1.00	13.42	C
ATOM	4141	O	LEU L	33	6.844	14.963	90.649	1.00	14.25	O
ATOM	4142	CB	LEU L	33	3.760	14.134	90.427	1.00	13.78	C
ATOM	4143	CG	LEU L	33	2.706	15.210	90.099	1.00	14.95	C
ATOM	4144	CD1	LEU L	33	3.156	16.597	90.519	1.00	12.91	C
ATOM	4145	CD2	LEU L	33	2.326	15.161	88.633	1.00	12.22	C
ATOM	4146	N	ALA L	34	5.877	16.121	88.978	1.00	11.33	N
ATOM	4147	CA	ALA L	34	6.769	17.253	89.086	1.00	6.84	C
ATOM	4148	C	ALA L	34	5.959	18.532	89.121	1.00	6.22	C
ATOM	4149	O	ALA L	34	4.767	18.528	88.809	1.00	7.58	O
ATOM	4150	CB	ALA L	34	7.697	17.262	87.908	1.00	5.43	C
ATOM	4151	N	TRP L	35	6.603	19.635	89.514	1.00	5.36	N

FIG. 53-67

ATOM	4153	C	TRP	L	35	6.924	21.966	89.048	1.00	3.47	C
ATOM	4154	O	TRP	L	35	8.061	22.052	89.515	1.00	3.50	O
ATOM	4155	CB	TRP	L	35	5.556	21.265	90.997	1.00	5.12	C
ATOM	4156	CG	TRP	L	35	4.297	20.596	91.453	1.00	4.90	C
ATOM	4157	CD1	TRP	L	35	4.195	19.500	92.251	1.00	4.38	C
ATOM	4158	CD2	TRP	L	35	2.954	21.036	91.202	1.00	3.51	C
ATOM	4159	NE1	TRP	L	35	2.879	19.238	92.524	1.00	2.89	N
ATOM	4160	CE2	TRP	L	35	2.099	20.163	91.895	1.00	2.00	C
ATOM	4161	CE3	TRP	L	35	2.400	22.083	90.464	1.00	3.91	C
ATOM	4162	CZ2	TRP	L	35	0.718	20.312	91.876	1.00	2.00	C
ATOM	4163	CZ3	TRP	L	35	1.021	22.228	90.448	1.00	2.00	C
ATOM	4164	CH2	TRP	L	35	0.198	21.347	91.149	1.00	2.38	C
ATOM	4165	N	TYR	L	36	6.470	22.740	88.064	1.00	4.17	N
ATOM	4166	CA	TYR	L	36	7.281	23.779	87.440	1.00	4.96	C
ATOM	4167	C	TYR	L	36	6.663	25.180	87.538	1.00	6.14	C
ATOM	4168	O	TYR	L	36	5.444	25.349	87.467	1.00	7.01	O
ATOM	4169	CB	TYR	L	36	7.525	23.442	85.973	1.00	3.09	C
ATOM	4170	CG	TYR	L	36	8.077	22.057	85.749	1.00	2.00	C
ATOM	4171	CD1	TYR	L	36	7.225	20.951	85.671	1.00	2.93	C
ATOM	4172	CD2	TYR	L	36	9.441	21.848	85.616	1.00	2.00	C
ATOM	4173	CE1	TYR	L	36	7.726	19.676	85.468	1.00	2.08	C
ATOM	4174	CE2	TYR	L	36	9.953	20.585	85.415	1.00	2.34	C
ATOM	4175	CZ	TYR	L	36	9.094	19.497	85.343	1.00	3.39	C
ATOM	4176	OH	TYR	L	36	9.610	18.233	85.179	1.00	2.55	O
ATOM	4177	N	GLN	L	37	7.520	26.178	87.696	1.00	5.95	N
ATOM	4178	CA	GLN	L	37	7.087	27.554	87.792	1.00	5.78	C
ATOM	4179	C	GLN	L	37	7.510	28.300	86.531	1.00	5.25	C
ATOM	4180	O	GLN	L	37	8.668	28.219	86.101	1.00	4.79	O
ATOM	4181	CB	GLN	L	37	7.728	28.216	89.016	1.00	6.32	C
ATOM	4182	CG	GLN	L	37	7.256	29.643	89.288	1.00	5.43	C
ATOM	4183	CD	GLN	L	37	8.156	30.369	90.261	1.00	4.23	C
ATOM	4184	OE1	GLN	L	37	9.372	30.468	90.052	1.00	4.94	O
ATOM	4185	NE2	GLN	L	37	7.569	30.901	91.317	1.00	2.38	N
ATOM	4186	N	GLN	L	38	6.590	29.018	85.915	1.00	4.82	N
ATOM	4187	CA	GLN	L	38	6.985	29.751	84.735	1.00	8.35	C
ATOM	4188	C	GLN	L	38	6.568	31.212	84.803	1.00	11.67	C
ATOM	4189	O	GLN	L	38	5.398	31.524	85.033	1.00	12.90	O
ATOM	4190	CB	GLN	L	38	6.451	29.101	83.452	1.00	7.29	C
ATOM	4191	CG	GLN	L	38	7.234	29.536	82.224	1.00	4.57	C
ATOM	4192	CD	GLN	L	38	6.624	29.084	80.933	1.00	3.14	C
ATOM	4193	OE1	GLN	L	38	5.463	28.700	80.893	1.00	3.34	O
ATOM	4194	NE2	GLN	L	38	7.395	29.148	79.858	1.00	2.00	N
ATOM	4195	N	LYS	L	39	7.552	32.097	84.685	1.00	12.62	N
ATOM	4196	CA	LYS	L	39	7.288	33.518	84.681	1.00	15.30	C
ATOM	4197	C	LYS	L	39	6.991	33.778	83.210	1.00	18.12	C
ATOM	4198	O	LYS	L	39	7.361	32.962	82.364	1.00	20.22	O
ATOM	4199	CB	LYS	L	39	8.529	34.282	85.130	1.00	15.46	C
ATOM	4200	CG	LYS	L	39	8.514	34.709	86.599	1.00	16.47	C
ATOM	4201	CD	LYS	L	39	8.613	33.536	87.561	1.00	16.42	C
ATOM	4202	CE	LYS	L	39	8.373	33.963	89.012	1.00	14.98	C
ATOM	4203	NZ	LYS	L	39	9.384	34.893	89.580	1.00	12.96	N
ATOM	4204	N	PRO	L	40	6.337	34.906	82.874	1.00	19.22	N
ATOM	4205	CA	PRO	L	40	6.002	35.242	81.487	1.00	20.79	C
ATOM	4206	C	PRO	L	40	6.847	34.650	80.340	1.00	21.94	C
ATOM	4207	O	PRO	L	40	6.514	33.568	79.823	1.00	23.08	O
ATOM	4208	CB	PRO	L	40	5.991	36.764	81.517	1.00	19.24	C
ATOM	4209	CG	PRO	L	40	5.262	37.005	82.793	1.00	18.51	C
ATOM	4210	CD	PRO	L	40	5.879	35.983	83.773	1.00	18.75	C
ATOM	4211	N	GLY	L	41	7.893	35.356	79.911	1.00	21.06	N
ATOM	4212	CA	GLY	L	41	8.712	34.847	78.820	1.00	20.00	C
ATOM	4213	C	GLY	L	41	9.974	34.121	79.261	1.00	18.97	C
ATOM	4214	O	GLY	L	41	11.030	34.252	78.633	1.00	19.04	O
ATOM	4215	N	GLN	L	42	9.874	33.335	80.326	1.00	16.60	N
ATOM	4216	CA	GLN	L	42	11.032	32.612	80.836	1.00	14.53	C
ATOM	4217	C	GLN	L	42	10.845	31.084	80.820	1.00	12.62	C
ATOM	4218	O	GLN	L	42	9.736	30.585	80.996	1.00	11.29	O
ATOM	4219	CB	GLN	L	42	11.320	33.048	82.270	1.00	16.46	C
ATOM	4220	CG	GLN	L	42	11.589	34.524	82.496	1.00	15.62	C
ATOM	4221	CD	GLN	L	42	12.004	34.799	83.937	1.00	16.42	C
ATOM	4222	OE1	GLN	L	42	12.068	33.886	84.756	1.00	14.59	O

FIG. 53-68

ATOM	4224	N	ALA	L	43	11.934	30.348	80.614	1.00	11.24	N
ATOM	4225	CA	ALA	L	43	11.905	28.890	80.620	1.00	11.00	C
ATOM	4226	C	ALA	L	43	11.442	28.460	82.005	1.00	12.34	C
ATOM	4227	O	ALA	L	43	11.689	29.172	82.987	1.00	13.78	O
ATOM	4228	CB	ALA	L	43	13.272	28.361	80.353	1.00	12.18	C
ATOM	4229	N	PRO	L	44	10.734	27.316	82.110	1.00	13.30	N
ATOM	4230	CA	PRO	L	44	10.233	26.818	83.404	1.00	11.61	C
ATOM	4231	C	PRO	L	44	11.269	26.510	84.486	1.00	11.74	C
ATOM	4232	O	PRO	L	44	12.406	26.119	84.199	1.00	10.92	O
ATOM	4233	CB	PRO	L	44	9.441	25.573	83.008	1.00	10.31	C
ATOM	4234	CG	PRO	L	44	8.920	25.933	81.645	1.00	9.78	C
ATOM	4235	CD	PRO	L	44	10.157	26.534	80.999	1.00	11.64	C
ATOM	4236	N	ARG	L	45	10.844	26.691	85.732	1.00	12.04	N
ATOM	4237	CA	ARG	L	45	11.670	26.450	86.911	1.00	12.58	C
ATOM	4238	C	ARG	L	45	11.185	25.191	87.614	1.00	10.42	C
ATOM	4239	O	ARG	L	45	10.041	25.152	88.059	1.00	10.54	O
ATOM	4240	CB	ARG	L	45	11.556	27.630	87.886	1.00	15.44	C
ATOM	4241	CG	ARG	L	45	12.550	28.760	87.653	1.00	20.75	C
ATOM	4242	CD	ARG	L	45	12.054	30.115	88.218	1.00	24.56	C
ATOM	4243	NE	ARG	L	45	11.048	30.748	87.355	1.00	21.85	N
ATOM	4244	CZ	ARG	L	45	11.279	31.154	86.104	1.00	21.74	C
ATOM	4245	NH1	ARG	L	45	12.486	31.009	85.562	1.00	22.07	N
ATOM	4246	NH2	ARG	L	45	10.289	31.651	85.368	1.00	19.12	N
ATOM	4247	N	LEU	L	46	12.049	24.175	87.709	1.00	8.36	N
ATOM	4248	CA	LEU	L	46	11.729	22.908	88.383	1.00	6.60	C
ATOM	4249	C	LEU	L	46	11.710	23.168	89.877	1.00	5.39	C
ATOM	4250	O	LEU	L	46	12.744	23.503	90.454	1.00	6.29	O
ATOM	4251	CB	LEU	L	46	12.797	21.844	88.064	1.00	6.01	C
ATOM	4252	CG	LEU	L	46	12.724	20.370	88.525	1.00	4.44	C
ATOM	4253	CD1	LEU	L	46	13.724	20.103	89.626	1.00	3.32	C
ATOM	4254	CD2	LEU	L	46	11.315	19.935	88.934	1.00	2.00	C
ATOM	4255	N	LEU	L	47	10.539	23.061	90.491	1.00	4.03	N
ATOM	4256	CA	LEU	L	47	10.425	23.301	91.925	1.00	4.61	C
ATOM	4257	C	LEU	L	47	10.514	22.005	92.699	1.00	6.13	C
ATOM	4258	O	LEU	L	47	11.352	21.858	93.593	1.00	6.17	O
ATOM	4259	CB	LEU	L	47	9.086	23.961	92.271	1.00	4.58	C
ATOM	4260	CG	LEU	L	47	8.644	25.279	91.630	1.00	4.25	C
ATOM	4261	CD1	LEU	L	47	7.228	25.577	92.075	1.00	2.00	C
ATOM	4262	CD2	LEU	L	47	9.598	26.419	91.994	1.00	2.00	C
ATOM	4263	N	ILE	L	48	9.664	21.054	92.315	1.00	6.44	N
ATOM	4264	CA	ILE	L	48	9.568	19.765	92.976	1.00	6.45	C
ATOM	4265	C	ILE	L	48	9.521	18.596	92.000	1.00	6.63	C
ATOM	4266	O	ILE	L	48	9.113	18.740	90.850	1.00	8.77	O
ATOM	4267	CB	ILE	L	48	8.314	19.764	93.888	1.00	6.82	C
ATOM	4268	CG1	ILE	L	48	8.553	20.714	95.067	1.00	6.46	C
ATOM	4269	CG2	ILE	L	48	7.972	18.362	94.372	1.00	6.08	C
ATOM	4270	CD1	ILE	L	48	7.345	21.008	95.869	1.00	6.38	C
ATOM	4271	N	TYR	L	49	9.996	17.444	92.447	1.00	7.79	N
ATOM	4272	CA	TYR	L	49	9.996	16.239	91.628	1.00	7.34	C
ATOM	4273	C	TYR	L	49	9.713	15.065	92.546	1.00	7.29	C
ATOM	4274	O	TYR	L	49	9.787	15.203	93.763	1.00	8.88	O
ATOM	4275	CB	TYR	L	49	11.339	16.061	90.913	1.00	7.81	C
ATOM	4276	CG	TYR	L	49	12.570	15.984	91.799	1.00	8.07	C
ATOM	4277	CD1	TYR	L	49	13.168	17.138	92.307	1.00	8.64	C
ATOM	4278	CD2	TYR	L	49	13.170	14.757	92.079	1.00	8.05	C
ATOM	4279	CE1	TYR	L	49	14.340	17.065	93.069	1.00	9.99	C
ATOM	4280	CE2	TYR	L	49	14.336	14.672	92.836	1.00	7.16	C
ATOM	4281	CZ	TYR	L	49	14.916	15.822	93.324	1.00	8.26	C
ATOM	4282	OH	TYR	L	49	16.085	15.714	94.042	1.00	10.59	O
ATOM	4283	N	GLY	L	50	9.365	13.924	91.977	1.00	5.39	N
ATOM	4284	CA	GLY	L	50	9.081	12.776	92.804	1.00	6.74	C
ATOM	4285	C	GLY	L	50	7.983	13.111	93.787	1.00	8.89	C
ATOM	4286	O	GLY	L	50	8.031	12.720	94.954	1.00	8.92	O
ATOM	4287	N	ALA	L	51	7.034	13.917	93.324	1.00	10.14	N
ATOM	4288	CA	ALA	L	51	5.884	14.344	94.110	1.00	9.53	C
ATOM	4289	C	ALA	L	51	6.142	15.215	95.337	1.00	10.33	C
ATOM	4290	O	ALA	L	51	5.328	16.085	95.639	1.00	11.66	O
ATOM	4291	CB	ALA	L	51	5.045	13.155	94.496	1.00	7.73	C
ATOM	4292	N	SER	L	52	7.276	15.049	96.010	1.00	9.61	N
ATOM	4293	CA	SER	L	52	7.513	15.811	97.728	1.00	9.93	C

FIG. 53-69

ATOM	4295	O	SER	L	52	9.137	16.985	98.518	1.00	13.47	O
ATOM	4296	CB	SER	L	52	7.048	14.980	98.425	1.00	8.86	C
ATOM	4297	OG	SER	L	52	7.734	13.737	98.471	1.00	6.01	O
ATOM	4298	N	THR	L	53	9.903	15.951	96.691	1.00	12.37	N
ATOM	4299	CA	THR	L	53	11.255	16.428	96.937	1.00	12.97	C
ATOM	4300	C	THR	L	53	11.543	17.688	96.142	1.00	15.00	C
ATOM	4301	O	THR	L	53	11.422	17.713	94.909	1.00	16.56	O
ATOM	4302	CB	THR	L	53	12.311	15.367	96.662	1.00	12.15	C
ATOM	4303	OG1	THR	L	53	13.615	15.951	96.785	1.00	13.42	O
ATOM	4304	CG2	THR	L	53	12.148	14.802	95.294	1.00	13.58	C
ATOM	4305	N	ARG	L	54	11.926	18.732	96.867	1.00	16.83	N
ATOM	4306	CA	ARG	L	54	12.213	20.044	96.295	1.00	16.86	C
ATOM	4307	C	ARG	L	54	13.607	20.133	95.664	1.00	16.76	C
ATOM	4308	O	ARG	L	54	14.566	19.549	96.184	1.00	15.87	O
ATOM	4309	CB	ARG	L	54	12.047	21.109	97.386	1.00	17.06	C
ATOM	4310	CG	ARG	L	54	10.812	20.896	98.265	1.00	17.51	C
ATOM	4311	CD	ARG	L	54	10.489	22.113	99.138	1.00	18.35	C
ATOM	4312	NE	ARG	L	54	11.659	22.614	99.851	1.00	18.71	N
ATOM	4313	CZ	ARG	L	54	12.000	22.248	101.083	1.00	19.95	C
ATOM	4314	NH1	ARG	L	54	11.249	21.382	101.753	1.00	18.43	N
ATOM	4315	NH2	ARG	L	54	13.118	22.717	101.629	1.00	21.61	N
ATOM	4316	N	ALA	L	55	13.715	20.903	94.580	1.00	16.45	N
ATOM	4317	CA	ALA	L	55	14.971	21.088	93.856	1.00	17.53	C
ATOM	4318	C	ALA	L	55	15.933	22.082	94.507	1.00	18.92	C
ATOM	4319	O	ALA	L	55	15.517	22.957	95.273	1.00	17.92	O
ATOM	4320	CB	ALA	L	55	14.691	21.498	92.440	1.00	18.04	C
ATOM	4321	N	THR	L	56	17.219	21.947	94.176	1.00	20.30	N
ATOM	4322	CA	THR	L	56	18.286	22.794	94.714	1.00	21.70	C
ATOM	4323	C	THR	L	56	18.025	24.293	94.587	1.00	22.13	C
ATOM	4324	O	THR	L	56	18.134	24.860	93.500	1.00	21.81	O
ATOM	4325	CB	THR	L	56	19.621	22.508	94.026	1.00	21.97	C
ATOM	4326	OG1	THR	L	56	19.713	21.118	93.694	1.00	25.18	O
ATOM	4327	CG2	THR	L	56	20.754	22.855	94.967	1.00	24.12	C
ATOM	4328	N	GLY	L	57	17.714	24.935	95.707	1.00	23.10	N
ATOM	4329	CA	GLY	L	57	17.451	26.366	95.686	1.00	22.60	C
ATOM	4330	C	GLY	L	57	15.966	26.683	95.597	1.00	22.62	C
ATOM	4331	O	GLY	L	57	15.564	27.684	94.998	1.00	23.70	O
ATOM	4332	N	VAL	L	58	15.148	25.816	96.183	1.00	20.52	N
ATOM	4333	CA	VAL	L	58	13.708	25.988	96.196	1.00	19.52	C
ATOM	4334	C	VAL	L	58	13.258	26.056	97.651	1.00	20.36	C
ATOM	4335	O	VAL	L	58	13.203	25.036	98.347	1.00	19.75	O
ATOM	4336	CB	VAL	L	58	12.995	24.814	95.479	1.00	19.08	C
ATOM	4337	CG1	VAL	L	58	11.481	24.943	95.606	1.00	19.49	C
ATOM	4338	CG2	VAL	L	58	13.389	24.784	94.016	1.00	18.19	C
ATOM	4339	N	PRO	L	59	12.967	27.270	98.142	1.00	21.45	N
ATOM	4340	CA	PRO	L	59	12.518	27.550	99.507	1.00	21.92	C
ATOM	4341	C	PRO	L	59	11.521	26.544	100.071	1.00	21.94	C
ATOM	4342	O	PRO	L	59	10.726	25.962	99.333	1.00	21.19	O
ATOM	4343	CB	PRO	L	59	11.887	28.926	99.360	1.00	22.93	C
ATOM	4344	CG	PRO	L	59	12.837	29.589	98.409	1.00	22.27	C
ATOM	4345	CD	PRO	L	59	13.072	28.519	97.364	1.00	22.63	C
ATOM	4346	N	ALA	L	60	11.554	26.374	101.394	1.00	22.13	N
ATOM	4347	CA	ALA	L	60	10.650	25.459	102.094	1.00	21.74	C
ATOM	4348	C	ALA	L	60	9.198	25.902	101.955	1.00	20.47	C
ATOM	4349	O	ALA	L	60	8.275	25.168	102.293	1.00	21.56	O
ATOM	4350	CB	ALA	L	60	11.030	25.378	103.545	1.00	23.21	C
ATOM	4351	N	ARG	L	61	9.041	27.139	101.498	1.00	20.42	N
ATOM	4352	CA	ARG	L	61	7.772	27.810	101.243	1.00	19.06	C
ATOM	4353	C	ARG	L	61	6.911	26.895	100.364	1.00	17.94	C
ATOM	4354	O	ARG	L	61	5.745	26.638	100.664	1.00	18.58	O
ATOM	4355	CB	ARG	L	61	8.098	29.103	100.482	1.00	19.44	C
ATOM	4356	CG	ARG	L	61	7.048	30.198	100.445	1.00	19.13	C
ATOM	4357	CD	ARG	L	61	7.504	31.296	99.459	1.00	19.17	C
ATOM	4358	NE	ARG	L	61	8.918	31.648	99.626	1.00	17.54	N
ATOM	4359	CZ	ARG	L	61	9.615	32.411	98.787	1.00	17.27	C
ATOM	4360	NH1	ARG	L	61	9.038	32.924	97.712	1.00	17.58	N
ATOM	4361	NH2	ARG	L	61	10.909	32.633	99.002	1.00	16.55	N
ATOM	4362	N	PHE	L	62	7.499	26.432	99.266	1.00	16.61	N
ATOM	4363	CA	PHE	L	62	6.822	25.548	98.327	1.00	14.88	C
ATOM	4364	C	PHE	L	62	6.977	24.140	98.933	1.00	14.11	C

FIG. 53-70

ATOM	4366	CB	PHE	L	62	7.561	25.540	96.980	1.00	14.31	C
ATOM	4367	CG	PHE	L	62	7.537	26.862	96.236	1.00	10.40	C
ATOM	4368	CD1	PHE	L	62	8.529	27.816	96.445	1.00	9.61	C
ATOM	4369	CD2	PHE	L	62	6.577	27.112	95.259	1.00	8.67	C
ATOM	4370	CE1	PHE	L	62	8.567	28.994	95.684	1.00	8.08	C
ATOM	4371	CE2	PHE	L	62	6.610	28.288	94.496	1.00	7.13	C
ATOM	4372	CZ	PHE	L	62	7.607	29.224	94.711	1.00	6.12	C
ATOM	4373	N	SER	L	63	5.796	23.388	98.805	1.00	12.89	N
ATOM	4374	CA	SER	L	63	5.754	22.033	99.342	1.00	12.61	C
ATOM	4375	C	SER	L	63	4.981	21.124	98.419	1.00	12.96	C
ATOM	4376	O	SER	L	63	3.998	21.550	97.811	1.00	13.82	O
ATOM	4377	CB	SER	L	63	5.117	22.008	100.736	1.00	14.31	C
ATOM	4378	OG	SER	L	63	6.075	22.307	101.739	1.00	17.32	O
ATOM	4379	N	GLY	L	64	5.445	19.880	98.303	1.00	13.07	N
ATOM	4380	CA	GLY	L	64	4.799	18.906	97.447	1.00	11.80	C
ATOM	4381	C	GLY	L	64	4.228	17.755	98.243	1.00	11.55	C
ATOM	4382	O	GLY	L	64	4.915	17.176	99.087	1.00	11.72	O
ATOM	4383	N	SER	L	65	2.974	17.413	97.974	1.00	11.43	N
ATOM	4384	CA	SER	L	65	2.318	16.323	98.674	1.00	12.21	C
ATOM	4385	C	SER	L	65	1.425	15.520	97.738	1.00	11.84	C
ATOM	4386	O	SER	L	65	1.031	16.008	96.672	1.00	10.30	O
ATOM	4387	CB	SER	L	65	1.471	16.889	99.808	1.00	13.44	C
ATOM	4388	OG	SER	L	65	0.446	17.714	99.286	1.00	17.96	O
ATOM	4389	N	GLY	L	66	1.119	14.290	98.143	1.00	12.20	N
ATOM	4390	CA	GLY	L	66	0.236	13.441	97.361	1.00	13.58	C
ATOM	4391	C	GLY	L	66	0.816	12.286	96.565	1.00	13.54	C
ATOM	4392	O	GLY	L	66	2.008	12.247	96.254	1.00	13.29	O
ATOM	4393	N	SER	L	67	-0.062	11.358	96.196	1.00	14.26	N
ATOM	4394	CA	SER	L	67	0.324	10.185	95.423	1.00	13.93	C
ATOM	4395	C	SER	L	67	-0.850	9.651	94.600	1.00	14.21	C
ATOM	4396	O	SER	L	67	-1.990	10.099	94.756	1.00	12.98	O
ATOM	4397	CB	SER	L	67	0.870	9.097	96.354	1.00	13.59	C
ATOM	4398	OG	SER	L	67	0.004	8.866	97.452	1.00	14.62	O
ATOM	4399	N	GLY	L	68	-0.561	8.702	93.713	1.00	15.44	N
ATOM	4400	CA	GLY	L	68	-1.598	8.117	92.891	1.00	15.85	C
ATOM	4401	C	GLY	L	68	-2.062	9.061	91.802	1.00	17.29	C
ATOM	4402	O	GLY	L	68	-1.300	9.356	90.876	1.00	17.46	O
ATOM	4403	N	ALA	L	69	-3.288	9.568	91.926	1.00	17.58	N
ATOM	4404	CA	ALA	L	69	-3.856	10.454	90.917	1.00	16.74	C
ATOM	4405	C	ALA	L	69	-4.374	11.810	91.415	1.00	17.31	C
ATOM	4406	O	ALA	L	69	-5.245	12.418	90.781	1.00	17.05	O
ATOM	4407	CB	ALA	L	69	-4.944	9.718	90.170	1.00	16.96	C
ATOM	4408	N	GLU	L	70	-3.834	12.283	92.535	1.00	17.00	N
ATOM	4409	CA	GLU	L	70	-4.217	13.573	93.116	1.00	18.39	C
ATOM	4410	C	GLU	L	70	-3.002	14.128	93.853	1.00	17.66	C
ATOM	4411	O	GLU	L	70	-2.471	13.487	94.763	1.00	17.23	O
ATOM	4412	CB	GLU	L	70	-5.395	13.410	94.090	1.00	20.10	C
ATOM	4413	CG	GLU	L	70	-5.791	14.683	94.865	1.00	22.93	C
ATOM	4414	CD	GLU	L	70	-6.442	15.770	93.999	1.00	23.97	C
ATOM	4415	OE1	GLU	L	70	-7.684	15.726	93.823	1.00	22.90	O
ATOM	4416	OE2	GLU	L	70	-5.721	16.683	93.521	1.00	21.68	O
ATOM	4417	N	PHE	L	71	-2.541	15.299	93.436	1.00	17.15	N
ATOM	4418	CA	PHE	L	71	-1.372	15.917	94.049	1.00	16.67	C
ATOM	4419	C	PHE	L	71	-1.693	17.361	94.447	1.00	15.90	C
ATOM	4420	O	PHE	L	71	-2.726	17.903	94.055	1.00	13.13	O
ATOM	4421	CB	PHE	L	71	-0.179	15.873	93.079	1.00	17.73	C
ATOM	4422	CG	PHE	L	71	0.061	14.512	92.449	1.00	17.75	C
ATOM	4423	CD1	PHE	L	71	-0.617	14.132	91.297	1.00	18.46	C
ATOM	4424	CD2	PHE	L	71	1.000	13.635	92.980	1.00	18.02	C
ATOM	4425	CE1	PHE	L	71	-0.350	12.895	90.683	1.00	18.94	C
ATOM	4426	CE2	PHE	L	71	1.269	12.400	92.374	1.00	15.52	C
ATOM	4427	CZ	PHE	L	71	0.594	12.035	91.225	1.00	15.95	C
ATOM	4428	N	THR	L	72	-0.826	17.965	95.256	1.00	17.14	N
ATOM	4429	CA	THR	L	72	-1.038	19.338	95.716	1.00	18.59	C
ATOM	4430	C	THR	L	72	0.308	20.030	95.850	1.00	18.60	C
ATOM	4431	O	THR	L	72	1.330	19.384	96.096	1.00	19.31	O
ATOM	4432	CB	THR	L	72	-1.731	19.401	97.105	1.00	19.45	C
ATOM	4433	OG1	THR	L	72	-2.449	18.191	97.362	1.00	23.15	O
ATOM	4434	CG2	THR	L	72	-2.728	20.537	97.143	1.00	20.85	C
ATOM	4435	N	LEU	L	73	0.300	21.343	95.661	1.00	18.01	N

FIG. 53-71

ATOM	4437	C	LEU	L	73	1.135	23.325	96.651	1.00	18.73	C
ATOM	4438	O	LEU	L	73	0.341	24.181	96.264	1.00	19.04	O
ATOM	4439	CB	LEU	L	73	1.931	22.654	94.378	1.00	13.93	C
ATOM	4440	CG	LEU	L	73	3.248	23.422	94.164	1.00	10.08	C
ATOM	4441	CD1	LEU	L	73	3.006	24.909	94.249	1.00	6.04	C
ATOM	4442	CD2	LEU	L	73	4.359	22.939	95.109	1.00	4.51	C
ATOM	4443	N	THR	L	74	1.677	23.327	97.862	1.00	19.96	N
ATOM	4444	CA	THR	L	74	1.413	24.378	98.823	1.00	21.66	C
ATOM	4445	C	THR	L	74	2.544	25.416	98.853	1.00	22.64	C
ATOM	4446	O	THR	L	74	3.727	25.062	98.788	1.00	24.72	O
ATOM	4447	CB	THR	L	74	1.236	23.766	100.233	1.00	22.41	C
ATOM	4448	OG1	THR	L	74	0.078	22.918	100.249	1.00	21.89	O
ATOM	4449	CG2	THR	L	74	1.084	24.855	101.289	1.00	22.57	C
ATOM	4450	N	ILE	L	75	2.176	26.693	98.902	1.00	21.64	N
ATOM	4451	CA	ILE	L	75	3.153	27.774	98.992	1.00	22.01	C
ATOM	4452	C	ILE	L	75	2.686	28.628	100.173	1.00	24.00	C
ATOM	4453	O	ILE	L	75	1.806	29.480	100.022	1.00	25.32	O
ATOM	4454	CB	ILE	L	75	3.182	28.662	97.737	1.00	19.75	C
ATOM	4455	CG1	ILE	L	75	3.278	27.810	96.470	1.00	18.53	C
ATOM	4456	CG2	ILE	L	75	4.372	29.614	97.814	1.00	16.78	C
ATOM	4457	CD1	ILE	L	75	3.065	28.592	95.192	1.00	14.90	C
ATOM	4458	N	SER	L	76	3.237	28.365	101.353	1.00	23.50	N
ATOM	4459	CA	SER	L	76	2.853	29.102	102.545	1.00	23.97	C
ATOM	4460	C	SER	L	76	2.974	30.618	102.378	1.00	24.28	C
ATOM	4461	O	SER	L	76	2.066	31.247	101.864	1.00	25.23	O
ATOM	4462	CB	SER	L	76	3.640	28.603	103.763	1.00	24.58	C
ATOM	4463	OG	SER	L	76	3.291	27.265	104.094	1.00	22.71	O
ATOM	4464	N	SER	L	77	4.090	31.200	102.787	1.00	25.69	N
ATOM	4465	CA	SER	L	77	4.274	32.643	102.672	1.00	26.77	C
ATOM	4466	C	SER	L	77	4.487	33.075	101.225	1.00	27.16	C
ATOM	4467	O	SER	L	77	5.613	33.020	100.727	1.00	28.12	O
ATOM	4468	CB	SER	L	77	5.480	33.087	103.508	1.00	28.35	C
ATOM	4469	OG	SER	L	77	6.670	32.393	103.132	1.00	29.03	O
ATOM	4470	N	LEU	L	78	3.410	33.476	100.547	1.00	26.54	N
ATOM	4471	CA	LEU	L	78	3.487	33.931	99.151	1.00	24.64	C
ATOM	4472	C	LEU	L	78	4.207	35.259	99.033	1.00	24.02	C
ATOM	4473	O	LEU	L	78	3.738	36.264	99.554	1.00	25.66	O
ATOM	4474	CB	LEU	L	78	2.092	34.126	98.583	1.00	23.31	C
ATOM	4475	CG	LEU	L	78	1.235	32.905	98.339	1.00	24.24	C
ATOM	4476	CD1	LEU	L	78	-0.206	33.342	98.363	1.00	26.17	C
ATOM	4477	CD2	LEU	L	78	1.602	32.265	97.017	1.00	23.99	C
ATOM	4478	N	GLN	L	79	5.331	35.289	98.337	1.00	23.25	N
ATOM	4479	CA	GLN	L	79	6.042	36.551	98.181	1.00	24.26	C
ATOM	4480	C	GLN	L	79	5.583	37.170	96.869	1.00	23.90	C
ATOM	4481	O	GLN	L	79	4.446	36.978	96.457	1.00	25.83	O
ATOM	4482	CB	GLN	L	79	7.555	36.330	98.193	1.00	25.76	C
ATOM	4483	CG	GLN	L	79	8.029	35.324	99.242	1.00	25.88	C
ATOM	4484	CD	GLN	L	79	7.585	35.657	100.648	1.00	25.29	C
ATOM	4485	OE1	GLN	L	79	6.394	35.731	100.936	1.00	23.42	O
ATOM	4486	NE2	GLN	L	79	8.546	35.858	101.535	1.00	27.79	N
ATOM	4487	N	SER	L	80	6.435	37.954	96.233	1.00	22.86	N
ATOM	4488	CA	SER	L	80	6.065	38.564	94.962	1.00	21.59	C
ATOM	4489	C	SER	L	80	6.785	37.772	93.889	1.00	19.35	C
ATOM	4490	O	SER	L	80	6.310	37.630	92.755	1.00	17.56	O
ATOM	4491	CB	SER	L	80	6.491	40.037	94.935	1.00	22.61	C
ATOM	4492	OG	SER	L	80	5.821	40.767	95.957	1.00	25.01	O
ATOM	4493	N	GLU	L	81	7.945	37.248	94.272	1.00	16.35	N
ATOM	4494	CA	GLU	L	81	8.757	36.439	93.379	1.00	15.26	C
ATOM	4495	C	GLU	L	81	7.963	35.202	92.932	1.00	13.47	C
ATOM	4496	O	GLU	L	81	8.163	34.694	91.832	1.00	13.42	O
ATOM	4497	CB	GLU	L	81	10.075	36.053	94.071	1.00	17.15	C
ATOM	4498	CG	GLU	L	81	10.052	36.176	95.614	1.00	21.02	C
ATOM	4499	CD	GLU	L	81	11.404	35.897	96.265	1.00	24.30	C
ATOM	4500	OE1	GLU	L	81	12.445	36.292	95.690	1.00	25.00	O
ATOM	4501	OE2	GLU	L	81	11.426	35.281	97.358	1.00	27.51	O
ATOM	4502	N	ASP	L	82	7.002	34.795	93.756	1.00	11.34	N
ATOM	4503	CA	ASP	L	82	6.156	33.638	93.485	1.00	10.32	C
ATOM	4504	C	ASP	L	82	5.016	33.905	92.511	1.00	9.98	C
ATOM	4505	O	ASP	L	82	4.026	33.171	92.514	1.00	8.00	O
ATOM	4506	CB	ASP	L	82	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

FIG. 53-72

ATOM	4508	OD1	ASP	L	82	7.804	32.822	95.533	1.00	15.38	O
ATOM	4509	OD2	ASP	L	82	6.201	32.798	97.037	1.00	14.01	O
ATOM	4510	N	PHE	L	83	5.093	35.003	91.759	1.00	10.15	N
ATOM	4511	CA	PHE	L	83	4.058	35.300	90.769	1.00	10.36	C
ATOM	4512	C	PHE	L	83	4.445	34.421	89.588	1.00	10.31	C
ATOM	4513	O	PHE	L	83	5.624	34.375	89.233	1.00	10.34	O
ATOM	4514	CB	PHE	L	83	4.088	36.785	90.348	1.00	12.04	C
ATOM	4515	CG	PHE	L	83	5.208	37.142	89.388	1.00	11.12	C
ATOM	4516	CD1	PHE	L	83	6.455	37.556	89.865	1.00	10.48	C
ATOM	4517	CD2	PHE	L	83	5.008	37.061	88.002	1.00	9.32	C
ATOM	4518	CE1	PHE	L	83	7.490	37.881	88.987	1.00	7.84	C
ATOM	4519	CE2	PHE	L	83	6.030	37.382	87.108	1.00	6.55	C
ATOM	4520	CZ	PHE	L	83	7.277	37.795	87.600	1.00	9.45	C
ATOM	4521	N	ALA	L	84	3.501	33.662	89.046	1.00	9.69	N
ATOM	4522	CA	ALA	L	84	3.775	32.800	87.893	1.00	10.39	C
ATOM	4523	C	ALA	L	84	2.671	31.789	87.674	1.00	10.20	C
ATOM	4524	O	ALA	L	84	1.648	31.799	88.384	1.00	10.33	O
ATOM	4525	CB	ALA	L	84	5.105	32.066	88.055	1.00	10.16	C
ATOM	4526	N	VAL	L	85	2.866	30.973	86.638	1.00	8.46	N
ATOM	4527	CA	VAL	L	85	1.947	29.904	86.282	1.00	7.17	C
ATOM	4528	C	VAL	L	85	2.655	28.652	86.785	1.00	7.11	C
ATOM	4529	O	VAL	L	85	3.887	28.567	86.706	1.00	7.67	O
ATOM	4530	CB	VAL	L	85	1.760	29.764	84.747	1.00	6.11	C
ATOM	4531	CG1	VAL	L	85	0.664	28.764	84.445	1.00	7.72	C
ATOM	4532	CG2	VAL	L	85	1.433	31.083	84.109	1.00	2.81	C
ATOM	4533	N	TYR	L	86	1.891	27.696	87.304	1.00	6.77	N
ATOM	4534	CA	TYR	L	86	2.449	26.447	87.824	1.00	5.61	C
ATOM	4535	C	TYR	L	86	1.930	25.291	87.008	1.00	6.30	C
ATOM	4536	O	TYR	L	86	0.756	25.276	86.630	1.00	7.74	O
ATOM	4537	CB	TYR	L	86	2.079	26.279	89.298	1.00	5.06	C
ATOM	4538	CG	TYR	L	86	2.806	27.282	90.151	1.00	4.06	C
ATOM	4539	CD1	TYR	L	86	2.281	28.558	90.369	1.00	4.49	C
ATOM	4540	CD2	TYR	L	86	4.076	27.001	90.640	1.00	5.08	C
ATOM	4541	CE1	TYR	L	86	3.015	29.532	91.046	1.00	5.20	C
ATOM	4542	CE2	TYR	L	86	4.815	27.963	91.312	1.00	6.83	C
ATOM	4543	CZ	TYR	L	86	4.286	29.224	91.513	1.00	5.62	C
ATOM	4544	OH	TYR	L	86	5.033	30.169	92.170	1.00	2.98	O
ATOM	4545	N	TYR	L	87	2.816	24.342	86.711	1.00	6.98	N
ATOM	4546	CA	TYR	L	87	2.488	23.166	85.909	1.00	5.96	C
ATOM	4547	C	TYR	L	87	2.916	21.887	86.607	1.00	5.99	C
ATOM	4548	O	TYR	L	87	3.976	21.846	87.215	1.00	7.08	O
ATOM	4549	CB	TYR	L	87	3.250	23.209	84.584	1.00	6.25	C
ATOM	4550	CG	TYR	L	87	2.854	24.294	83.614	1.00	6.20	C
ATOM	4551	CD1	TYR	L	87	1.660	24.218	82.902	1.00	7.29	C
ATOM	4552	CD2	TYR	L	87	3.712	25.360	83.349	1.00	8.25	C
ATOM	4553	CE1	TYR	L	87	1.331	25.169	81.945	1.00	7.18	C
ATOM	4554	CE2	TYR	L	87	3.391	26.313	82.392	1.00	8.23	C
ATOM	4555	CZ	TYR	L	87	2.203	26.207	81.691	1.00	8.35	C
ATOM	4556	OH	TYR	L	87	1.925	27.106	80.693	1.00	12.74	O
ATOM	4557	N	CYS	L	88	2.139	20.824	86.442	1.00	6.86	N
ATOM	4558	CA	CYS	L	88	2.469	19.526	87.028	1.00	7.91	C
ATOM	4559	C	CYS	L	88	2.677	18.544	85.883	1.00	8.19	C
ATOM	4560	O	CYS	L	88	1.929	18.553	84.910	1.00	8.52	O
ATOM	4561	CB	CYS	L	88	1.352	19.036	87.941	1.00	8.00	C
ATOM	4562	SG	CYS	L	88	-0.208	18.550	87.117	1.00	14.73	S
ATOM	4563	N	GLN	L	89	3.698	17.704	85.988	1.00	9.10	N
ATOM	4564	CA	GLN	L	89	3.990	16.736	84.935	1.00	10.07	C
ATOM	4565	C	GLN	L	89	4.237	15.341	85.473	1.00	11.75	C
ATOM	4566	O	GLN	L	89	5.076	15.151	86.357	1.00	13.16	O
ATOM	4567	CB	GLN	L	89	5.222	17.173	84.140	1.00	7.86	C
ATOM	4568	CG	GLN	L	89	5.767	16.106	83.207	1.00	3.60	C
ATOM	4569	CD	GLN	L	89	7.268	16.200	83.025	1.00	3.91	C
ATOM	4570	OE1	GLN	L	89	7.808	15.788	82.000	1.00	5.27	O
ATOM	4571	NE2	GLN	L	89	7.956	16.727	84.031	1.00	2.00	N
ATOM	4572	N	GLN	L	90	3.529	14.364	84.919	1.00	13.92	N
ATOM	4573	CA	GLN	L	90	3.704	12.976	85.329	1.00	14.37	C
ATOM	4574	C	GLN	L	90	4.740	12.358	84.409	1.00	14.11	C
ATOM	4575	O	GLN	L	90	4.878	12.760	83.252	1.00	14.22	O
ATOM	4576	CB	GLN	L	90	2.384	12.206	85.209	1.00	16.09	C
ATOM	4577	CG	GLN	L	90	1.894	11.934	83.783	1.00	18.12	C

FIG. 53-73

ATOM	4579	OE1	GLN	L	90	2.745	10.772	81.861	1.00	19.12	O
ATOM	4580	NE2	GLN	L	90	3.161	9.868	83.870	1.00	21.14	N
ATOM	4581	N	TYR	L	91	5.436	11.345	84.898	1.00	14.31	N
ATOM	4582	CA	TYR	L	91	6.439	10.663	84.085	1.00	14.21	C
ATOM	4583	C	TYR	L	91	6.583	9.230	84.563	1.00	12.81	C
ATOM	4584	O	TYR	L	91	7.680	8.684	84.595	1.00	12.62	O
ATOM	4585	CB	TYR	L	91	7.792	11.404	84.117	1.00	14.56	C
ATOM	4586	CG	TYR	L	91	8.262	11.779	85.501	1.00	14.78	C
ATOM	4587	CD1	TYR	L	91	7.777	12.926	86.132	1.00	15.04	C
ATOM	4588	CD2	TYR	L	91	9.138	10.963	86.206	1.00	14.16	C
ATOM	4589	CE1	TYR	L	91	8.125	13.232	87.427	1.00	13.42	C
ATOM	4590	CE2	TYR	L	91	9.495	11.266	87.517	1.00	15.16	C
ATOM	4591	CZ	TYR	L	91	8.981	12.405	88.117	1.00	14.10	C
ATOM	4592	OH	TYR	L	91	9.275	12.701	89.421	1.00	12.42	O
ATOM	4593	N	ASN	L	92	5.456	8.631	84.921	1.00	12.06	N
ATOM	4594	CA	ASN	L	92	5.441	7.259	85.409	1.00	13.38	C
ATOM	4595	C	ASN	L	92	5.662	6.243	84.302	1.00	13.10	C
ATOM	4596	O	ASN	L	92	6.606	5.453	84.364	1.00	14.86	O
ATOM	4597	CB	ASN	L	92	4.124	6.962	86.123	1.00	13.96	C
ATOM	4598	CG	ASN	L	92	4.114	5.591	86.781	1.00	16.48	C
ATOM	4599	OD1	ASN	L	92	3.139	4.846	86.671	1.00	17.04	O
ATOM	4600	ND2	ASN	L	92	5.188	5.264	87.489	1.00	18.14	N
ATOM	4601	N	ASN	L	93	4.805	6.305	83.280	1.00	11.53	N
ATOM	4602	CA	ASN	L	93	4.833	5.404	82.125	1.00	8.54	C
ATOM	4603	C	ASN	L	93	6.136	5.120	81.379	1.00	7.78	C
ATOM	4604	O	ASN	L	93	7.072	5.911	81.387	1.00	6.63	O
ATOM	4605	CB	ASN	L	93	3.749	5.798	81.110	1.00	7.89	C
ATOM	4606	CG	ASN	L	93	3.803	7.271	80.699	1.00	6.74	C
ATOM	4607	OD1	ASN	L	93	2.901	7.754	80.029	1.00	8.49	O
ATOM	4608	ND2	ASN	L	93	4.861	7.973	81.072	1.00	6.95	N
ATOM	4609	N	TRP	L	94	6.180	3.943	80.765	1.00	8.55	N
ATOM	4610	CA	TRP	L	94	7.319	3.495	79.973	1.00	8.39	C
ATOM	4611	C	TRP	L	94	6.777	2.509	78.928	1.00	10.86	C
ATOM	4612	O	TRP	L	94	6.035	1.585	79.276	1.00	13.10	O
ATOM	4613	CB	TRP	L	94	8.381	2.829	80.834	1.00	4.60	C
ATOM	4614	CG	TRP	L	94	9.621	2.575	80.051	1.00	5.78	C
ATOM	4615	CD1	TRP	L	94	9.845	1.543	79.189	1.00	5.72	C
ATOM	4616	CD2	TRP	L	94	10.754	3.450	79.929	1.00	6.84	C
ATOM	4617	NE1	TRP	L	94	11.032	1.729	78.523	1.00	6.91	N
ATOM	4618	CE2	TRP	L	94	11.610	2.893	78.956	1.00	7.01	C
ATOM	4619	CE3	TRP	L	94	11.118	4.660	80.534	1.00	8.34	C
ATOM	4620	CZ2	TRP	L	94	12.808	3.502	78.572	1.00	6.29	C
ATOM	4621	CZ3	TRP	L	94	12.309	5.268	80.150	1.00	10.04	C
ATOM	4622	CH2	TRP	L	94	13.138	4.684	79.175	1.00	8.04	C
ATOM	4623	N	PRO	L	95	7.102	2.711	77.631	1.00	12.64	N
ATOM	4624	CA	PRO	L	95	7.906	3.796	77.035	1.00	12.43	C
ATOM	4625	C	PRO	L	95	7.390	5.174	77.417	1.00	11.48	C
ATOM	4626	O	PRO	L	95	6.185	5.353	77.619	1.00	13.24	O
ATOM	4627	CB	PRO	L	95	7.759	3.554	75.533	1.00	10.88	C
ATOM	4628	CG	PRO	L	95	7.546	2.072	75.450	1.00	12.47	C
ATOM	4629	CD	PRO	L	95	6.586	1.813	76.581	1.00	10.61	C
ATOM	4630	N	PRO	L	96	8.293	6.156	77.528	1.00	10.03	N
ATOM	4631	CA	PRO	L	96	7.989	7.541	77.888	1.00	8.83	C
ATOM	4632	C	PRO	L	96	6.846	8.185	77.108	1.00	9.51	C
ATOM	4633	O	PRO	L	96	6.860	8.267	75.887	1.00	9.25	O
ATOM	4634	CB	PRO	L	96	9.308	8.251	77.614	1.00	7.78	C
ATOM	4635	CG	PRO	L	96	10.307	7.225	77.935	1.00	8.31	C
ATOM	4636	CD	PRO	L	96	9.735	5.995	77.277	1.00	9.84	C
ATOM	4637	N	ARG	L	97	5.831	8.609	77.840	1.00	11.51	N
ATOM	4638	CA	ARG	L	97	4.683	9.289	77.278	1.00	12.61	C
ATOM	4639	C	ARG	L	97	4.309	10.253	78.397	1.00	12.40	C
ATOM	4640	O	ARG	L	97	3.150	10.333	78.823	1.00	12.94	O
ATOM	4641	CB	ARG	L	97	3.556	8.302	77.017	1.00	17.09	C
ATOM	4642	CG	ARG	L	97	3.857	7.269	75.947	1.00	22.39	C
ATOM	4643	CD	ARG	L	97	2.971	6.037	76.132	1.00	26.24	C
ATOM	4644	NE	ARG	L	97	3.286	5.283	77.346	1.00	28.09	N
ATOM	4645	CZ	ARG	L	97	3.788	4.054	77.352	1.00	28.60	C
ATOM	4646	NH1	ARG	L	97	4.040	3.434	76.209	1.00	30.10	N
ATOM	4647	NH2	ARG	L	97	4.023	3.439	78.499	1.00	29.71	N
ATOM	4648	N	TYR	L	98	5.345	10.918	78.912	1.00	11.60	N

FIG. 53-74

ATOM	4650	C	TYR	L	98	4.363	13.058	79.558	1.00	11.64	C
ATOM	4651	O	TYR	L	98	4.478	13.527	78.421	1.00	13.48	O
ATOM	4652	CB	TYR	L	98	6.636	12.364	80.400	1.00	12.53	C
ATOM	4653	CG	TYR	L	98	7.664	11.252	80.600	1.00	13.17	C
ATOM	4654	CD1	TYR	L	98	7.276	9.916	80.785	1.00	10.99	C
ATOM	4655	CD2	TYR	L	98	9.035	11.543	80.599	1.00	14.00	C
ATOM	4656	CE1	TYR	L	98	8.229	8.897	80.961	1.00	9.87	C
ATOM	4657	CE2	TYR	L	98	9.993	10.534	80.780	1.00	14.26	C
ATOM	4658	CZ	TYR	L	98	9.582	9.212	80.958	1.00	13.39	C
ATOM	4659	OH	TYR	L	98	10.531	8.229	81.125	1.00	8.87	O
ATOM	4660	N	THR	L	99	3.493	13.536	80.439	1.00	9.53	N
ATOM	4661	CA	THR	L	99	2.573	14.609	80.067	1.00	9.79	C
ATOM	4662	C	THR	L	99	2.517	15.767	81.051	1.00	9.59	C
ATOM	4663	O	THR	L	99	2.939	15.640	82.198	1.00	9.97	O
ATOM	4664	CB	THR	L	99	1.127	14.042	79.884	1.00	12.13	C
ATOM	4665	OG1	THR	L	99	0.721	13.338	81.072	1.00	10.31	O
ATOM	4666	CG2	THR	L	99	1.065	13.079	78.692	1.00	11.41	C
ATOM	4667	N	PHE	L	100	1.964	16.889	80.601	1.00	10.05	N
ATOM	4668	CA	PHE	L	100	1.822	18.087	81.430	1.00	7.56	C
ATOM	4669	C	PHE	L	100	0.360	18.422	81.683	1.00	8.42	C
ATOM	4670	O	PHE	L	100	-0.547	17.900	81.012	1.00	6.96	O
ATOM	4671	CB	PHE	L	100	2.443	19.297	80.738	1.00	4.66	C
ATOM	4672	CG	PHE	L	100	3.932	19.339	80.795	1.00	3.07	C
ATOM	4673	CD1	PHE	L	100	4.694	18.736	79.812	1.00	5.57	C
ATOM	4674	CD2	PHE	L	100	4.575	20.000	81.827	1.00	2.00	C
ATOM	4675	CE1	PHE	L	100	6.090	18.792	79.857	1.00	6.31	C
ATOM	4676	CE2	PHE	L	100	5.955	20.062	81.884	1.00	2.00	C
ATOM	4677	CZ	PHE	L	100	6.718	19.458	80.899	1.00	3.05	C
ATOM	4678	N	GLY	L	101	0.144	19.279	82.673	1.00	9.22	N
ATOM	4679	CA	GLY	L	101	-1.191	19.749	82.987	1.00	10.55	C
ATOM	4680	C	GLY	L	101	-1.278	21.122	82.336	1.00	11.54	C
ATOM	4681	O	GLY	L	101	-0.242	21.720	82.025	1.00	10.78	O
ATOM	4682	N	GLN	L	102	-2.490	21.640	82.145	1.00	13.06	N
ATOM	4683	CA	GLN	L	102	-2.669	22.948	81.515	1.00	13.20	C
ATOM	4684	C	GLN	L	102	-2.292	24.155	82.397	1.00	12.85	C
ATOM	4685	O	GLN	L	102	-2.497	25.310	82.011	1.00	12.27	O
ATOM	4686	CB	GLN	L	102	-4.095	23.093	80.972	1.00	14.24	C
ATOM	4687	CG	GLN	L	102	-5.117	23.675	81.947	1.00	15.34	C
ATOM	4688	CD	GLN	L	102	-5.437	22.758	83.107	1.00	16.33	C
ATOM	4689	OE1	GLN	L	102	-4.986	21.602	83.155	1.00	14.14	O
ATOM	4690	NE2	GLN	L	102	-6.206	23.275	84.069	1.00	14.33	N
ATOM	4691	N	GLY	L	103	-1.759	23.882	83.582	1.00	12.36	N
ATOM	4692	CA	GLY	L	103	-1.343	24.946	84.475	1.00	12.60	C
ATOM	4693	C	GLY	L	103	-2.389	25.690	85.285	1.00	12.40	C
ATOM	4694	O	GLY	L	103	-3.561	25.765	84.909	1.00	13.24	O
ATOM	4695	N	THR	L	104	-1.938	26.228	86.414	1.00	11.51	N
ATOM	4696	CA	THR	L	104	-2.757	27.013	87.330	1.00	11.59	C
ATOM	4697	C	THR	L	104	-2.092	28.388	87.324	1.00	10.45	C
ATOM	4698	O	THR	L	104	-0.864	28.466	87.408	1.00	10.03	O
ATOM	4699	CB	THR	L	104	-2.712	26.423	88.767	1.00	13.28	C
ATOM	4700	OG1	THR	L	104	-3.350	25.137	88.778	1.00	16.79	O
ATOM	4701	CG2	THR	L	104	-3.419	27.338	89.769	1.00	13.46	C
ATOM	4702	N	ARG	L	105	-2.875	29.449	87.112	1.00	9.53	N
ATOM	4703	CA	ARG	L	105	-2.347	30.816	87.092	1.00	10.17	C
ATOM	4704	C	ARG	L	105	-2.426	31.411	88.487	1.00	8.72	C
ATOM	4705	O	ARG	L	105	-3.518	31.591	89.019	1.00	6.15	O
ATOM	4706	CB	ARG	L	105	-3.155	31.694	86.139	1.00	13.45	C
ATOM	4707	CG	ARG	L	105	-2.867	31.481	84.655	1.00	18.32	C
ATOM	4708	CD	ARG	L	105	-4.156	31.289	83.851	1.00	18.07	C
ATOM	4709	NE	ARG	L	105	-4.578	29.894	83.843	1.00	16.55	N
ATOM	4710	CZ	ARG	L	105	-4.026	28.966	83.071	1.00	21.31	C
ATOM	4711	NH1	ARG	L	105	-3.029	29.295	82.247	1.00	21.54	N
ATOM	4712	NH2	ARG	L	105	-4.455	27.707	83.127	1.00	24.25	N
ATOM	4713	N	LEU	L	106	-1.277	31.728	89.074	1.00	9.90	N
ATOM	4714	CA	LEU	L	106	-1.245	32.285	90.426	1.00	12.46	C
ATOM	4715	C	LEU	L	106	-1.020	33.805	90.440	1.00	12.71	C
ATOM	4716	O	LEU	L	106	0.115	34.271	90.356	1.00	12.95	O
ATOM	4717	CB	LEU	L	106	-0.172	31.576	91.260	1.00	12.39	C
ATOM	4718	CG	LEU	L	106	-0.065	32.022	92.726	1.00	13.06	C
ATOM	4719	CD1	LEU	L	106	1.407	31.857	93.417	1.00	9.96	C

FIG. 53-75

ATOM	4721	N	GLU	L	107	-2.101	34.565	90.582	1.00	13.08	N
ATOM	4722	CA	GLU	L	107	-2.013	36.017	90.589	1.00	14.42	C
ATOM	4723	C	GLU	L	107	-2.267	36.679	91.951	1.00	15.47	C
ATOM	4724	O	GLU	L	107	-2.788	36.054	92.893	1.00	14.67	O
ATOM	4725	CB	GLU	L	107	-2.953	36.600	89.543	1.00	14.27	C
ATOM	4726	CG	GLU	L	107	-4.399	36.226	89.770	1.00	14.41	C
ATOM	4727	CD	GLU	L	107	-5.297	37.432	89.928	1.00	14.83	C
ATOM	4728	OE1	GLU	L	107	-5.148	38.404	89.161	1.00	15.25	O
ATOM	4729	OE2	GLU	L	107	-6.162	37.405	90.822	1.00	14.96	O
ATOM	4730	N	ILE	L	108	-1.897	37.961	92.021	1.00	15.44	N
ATOM	4731	CA	ILE	L	108	-2.022	38.796	93.217	1.00	12.47	C
ATOM	4732	C	ILE	L	108	-3.435	39.342	93.374	1.00	12.47	C
ATOM	4733	O	ILE	L	108	-3.965	39.993	92.468	1.00	11.83	O
ATOM	4734	CB	ILE	L	108	-1.067	40.007	93.148	1.00	11.33	C
ATOM	4735	CG1	ILE	L	108	0.359	39.544	92.842	1.00	8.42	C
ATOM	4736	CG2	ILE	L	108	-1.130	40.784	94.447	1.00	11.29	C
ATOM	4737	CD1	ILE	L	108	1.342	40.645	92.658	1.00	8.08	C
ATOM	4738	N	LYS	L	109	-4.040	39.079	94.528	1.00	12.15	N
ATOM	4739	CA	LYS	L	109	-5.384	39.555	94.803	1.00	12.07	C
ATOM	4740	C	LYS	L	109	-5.281	40.868	95.566	1.00	13.37	C
ATOM	4741	O	LYS	L	109	-4.522	40.976	96.531	1.00	14.27	O
ATOM	4742	CB	LYS	L	109	-6.168	38.539	95.634	1.00	10.80	C
ATOM	4743	CG	LYS	L	109	-7.660	38.849	95.710	1.00	10.92	C
ATOM	4744	CD	LYS	L	109	-8.262	38.428	97.030	1.00	11.47	C
ATOM	4745	CE	LYS	L	109	-8.214	36.937	97.205	1.00	14.99	C
ATOM	4746	NZ	LYS	L	109	-8.792	36.548	98.511	1.00	17.24	N
ATOM	4747	N	ARG	L	110	-6.031	41.866	95.124	1.00	13.56	N
ATOM	4748	CA	ARG	L	110	-6.031	43.169	95.768	1.00	13.88	C
ATOM	4749	C	ARG	L	110	-7.455	43.693	95.698	1.00	14.01	C
ATOM	4750	O	ARG	L	110	-8.385	42.927	95.436	1.00	14.87	O
ATOM	4751	CB	ARG	L	110	-5.078	44.124	95.048	1.00	14.70	C
ATOM	4752	CG	ARG	L	110	-5.293	44.201	93.553	1.00	17.17	C
ATOM	4753	CD	ARG	L	110	-4.842	45.537	92.996	1.00	20.25	C
ATOM	4754	NE	ARG	L	110	-5.734	46.629	93.378	1.00	22.67	N
ATOM	4755	CZ	ARG	L	110	-5.412	47.919	93.308	1.00	24.63	C
ATOM	4756	NH1	ARG	L	110	-4.211	48.294	92.872	1.00	25.47	N
ATOM	4757	NH2	ARG	L	110	-6.296	48.839	93.676	1.00	24.14	N
ATOM	4758	N	THR	L	111	-7.642	44.979	95.961	1.00	13.27	N
ATOM	4759	CA	THR	L	111	-8.980	45.552	95.901	1.00	12.64	C
ATOM	4760	C	THR	L	111	-9.415	45.912	94.480	1.00	12.65	C
ATOM	4761	O	THR	L	111	-8.590	46.132	93.581	1.00	12.06	O
ATOM	4762	CB	THR	L	111	-9.134	46.786	96.830	1.00	10.77	C
ATOM	4763	OG1	THR	L	111	-7.977	47.627	96.726	1.00	9.50	O
ATOM	4764	CG2	THR	L	111	-9.312	46.340	98.269	1.00	11.72	C
ATOM	4765	N	VAL	L	112	-10.726	45.947	94.291	1.00	12.84	N
ATOM	4766	CA	VAL	L	112	-11.322	46.282	93.018	1.00	14.13	C
ATOM	4767	C	VAL	L	112	-11.036	47.735	92.676	1.00	14.88	C
ATOM	4768	O	VAL	L	112	-11.193	48.634	93.508	1.00	17.13	O
ATOM	4769	CB	VAL	L	112	-12.844	46.059	93.066	1.00	15.42	C
ATOM	4770	CG1	VAL	L	112	-13.497	46.510	91.765	1.00	13.79	C
ATOM	4771	CG2	VAL	L	112	-13.140	44.590	93.360	1.00	14.81	C
ATOM	4772	N	ALA	L	113	-10.612	47.946	91.443	1.00	14.08	N
ATOM	4773	CA	ALA	L	113	-10.290	49.263	90.930	1.00	11.78	C
ATOM	4774	C	ALA	L	113	-10.817	49.317	89.504	1.00	11.36	C
ATOM	4775	O	ALA	L	113	-10.383	48.544	88.649	1.00	11.74	O
ATOM	4776	CB	ALA	L	113	-8.774	49.462	90.938	1.00	9.94	C
ATOM	4777	N	ALA	L	114	-11.789	50.188	89.263	1.00	11.49	N
ATOM	4778	CA	ALA	L	114	-12.382	50.349	87.931	1.00	10.65	C
ATOM	4779	C	ALA	L	114	-11.345	50.830	86.924	1.00	10.71	C
ATOM	4780	O	ALA	L	114	-10.319	51.378	87.309	1.00	10.78	O
ATOM	4781	CB	ALA	L	114	-13.543	51.330	87.990	1.00	8.85	C
ATOM	4782	N	PRO	L	115	-11.567	50.556	85.624	1.00	12.64	N
ATOM	4783	CA	PRO	L	115	-10.646	50.971	84.558	1.00	13.53	C
ATOM	4784	C	PRO	L	115	-10.870	52.386	84.047	1.00	14.19	C
ATOM	4785	O	PRO	L	115	-12.002	52.846	83.938	1.00	15.12	O
ATOM	4786	CB	PRO	L	115	-10.921	49.949	83.456	1.00	14.01	C
ATOM	4787	CG	PRO	L	115	-12.370	49.662	83.627	1.00	13.50	C
ATOM	4788	CD	PRO	L	115	-12.509	49.537	85.123	1.00	12.92	C
ATOM	4789	N	SER	L	116	-9.779	53.080	83.751	1.00	15.47	N
ATOM	4790	CA	SER	L	116	-9.847	54.429	83.214	1.00	15.68	C

FIG. 53-76

ATOM	4792	O	SER	L	116	-8.903	53.937	81.078	1.00	18.27	O
ATOM	4793	CB	SER	L	116	-8.580	55.212	83.568	1.00	15.35	C
ATOM	4794	OG	SER	L	116	-8.371	55.226	84.972	1.00	15.79	O
ATOM	4795	N	VAL	L	117	-11.136	54.218	81.181	1.00	16.94	N
ATOM	4796	CA	VAL	L	117	-11.356	53.979	79.755	1.00	16.67	C
ATOM	4797	C	VAL	L	117	-10.901	55.136	78.862	1.00	17.18	C
ATOM	4798	O	VAL	L	117	-10.979	56.307	79.250	1.00	18.64	O
ATOM	4799	CB	VAL	L	117	-12.840	53.652	79.481	1.00	16.30	C
ATOM	4800	CG1	VAL	L	117	-13.031	53.215	78.038	1.00	17.39	C
ATOM	4801	CG2	VAL	L	117	-13.317	52.565	80.439	1.00	12.57	C
ATOM	4802	N	PHE	L	118	-10.394	54.803	77.680	1.00	16.97	N
ATOM	4803	CA	PHE	L	118	-9.928	55.800	76.720	1.00	16.16	C
ATOM	4804	C	PHE	L	118	-10.135	55.272	75.305	1.00	16.79	C
ATOM	4805	O	PHE	L	118	-9.853	54.112	75.030	1.00	17.04	O
ATOM	4806	CB	PHE	L	118	-8.444	56.094	76.928	1.00	15.58	C
ATOM	4807	CG	PHE	L	118	-8.118	56.652	78.279	1.00	16.00	C
ATOM	4808	CD1	PHE	L	118	-8.615	57.892	78.675	1.00	16.23	C
ATOM	4809	CD2	PHE	L	118	-7.316	55.933	79.163	1.00	14.89	C
ATOM	4810	CE1	PHE	L	118	-8.323	58.409	79.933	1.00	14.96	C
ATOM	4811	CE2	PHE	L	118	-7.016	56.438	80.420	1.00	14.32	C
ATOM	4812	CZ	PHE	L	118	-7.521	57.682	80.808	1.00	16.00	C
ATOM	4813	N	ILE	L	119	-10.640	56.117	74.412	1.00	16.97	N
ATOM	4814	CA	ILE	L	119	-10.867	55.710	73.033	1.00	18.14	C
ATOM	4815	C	ILE	L	119	-9.896	56.477	72.135	1.00	18.40	C
ATOM	4816	O	ILE	L	119	-9.322	57.490	72.558	1.00	18.80	O
ATOM	4817	CB	ILE	L	119	-12.340	55.958	72.594	1.00	17.61	C
ATOM	4818	CG1	ILE	L	119	-12.703	55.036	71.430	1.00	15.98	C
ATOM	4819	CG2	ILE	L	119	-12.550	57.413	72.181	1.00	19.09	C
ATOM	4820	CD1	ILE	L	119	-14.149	55.164	70.973	1.00	16.09	C
ATOM	4821	N	PHE	L	120	-9.677	55.961	70.928	1.00	18.54	N
ATOM	4822	CA	PHE	L	120	-8.773	56.576	69.957	1.00	19.20	C
ATOM	4823	C	PHE	L	120	-9.305	56.406	68.533	1.00	19.76	C
ATOM	4824	O	PHE	L	120	-9.706	55.312	68.149	1.00	21.23	O
ATOM	4825	CB	PHE	L	120	-7.378	55.939	70.023	1.00	16.85	C
ATOM	4826	CG	PHE	L	120	-6.653	56.159	71.324	1.00	16.80	C
ATOM	4827	CD1	PHE	L	120	-6.334	57.450	71.756	1.00	15.81	C
ATOM	4828	CD2	PHE	L	120	-6.226	55.069	72.092	1.00	15.45	C
ATOM	4829	CE1	PHE	L	120	-5.592	57.652	72.937	1.00	15.59	C
ATOM	4830	CE2	PHE	L	120	-5.486	55.259	73.274	1.00	15.71	C
ATOM	4831	CZ	PHE	L	120	-5.167	56.549	73.696	1.00	14.12	C
ATOM	4832	N	PRO	L	121	-9.424	57.509	67.779	1.00	20.16	N
ATOM	4833	CA	PRO	L	121	-9.912	57.430	66.401	1.00	21.06	C
ATOM	4834	C	PRO	L	121	-8.778	56.938	65.504	1.00	20.94	C
ATOM	4835	O	PRO	L	121	-7.620	56.947	65.913	1.00	20.50	O
ATOM	4836	CB	PRO	L	121	-10.257	58.890	66.082	1.00	21.51	C
ATOM	4837	CG	PRO	L	121	-10.567	59.482	67.416	1.00	21.20	C
ATOM	4838	CD	PRO	L	121	-9.470	58.901	68.262	1.00	20.05	C
ATOM	4839	N	PRO	L	122	-9.098	56.463	64.287	1.00	22.00	N
ATOM	4840	CA	PRO	L	122	-8.067	55.978	63.360	1.00	22.92	C
ATOM	4841	C	PRO	L	122	-7.288	57.181	62.836	1.00	23.88	C
ATOM	4842	O	PRO	L	122	-7.871	58.112	62.285	1.00	24.51	O
ATOM	4843	CB	PRO	L	122	-8.885	55.337	62.235	1.00	22.26	C
ATOM	4844	CG	PRO	L	122	-10.181	54.978	62.887	1.00	22.25	C
ATOM	4845	CD	PRO	L	122	-10.441	56.183	63.759	1.00	22.67	C
ATOM	4846	N	SER	L	123	-5.973	57.158	63.005	1.00	25.66	N
ATOM	4847	CA	SER	L	123	-5.112	58.252	62.571	1.00	26.94	C
ATOM	4848	C	SER	L	123	-5.327	58.635	61.115	1.00	28.60	C
ATOM	4849	O	SER	L	123	-5.534	57.773	60.259	1.00	28.79	O
ATOM	4850	CB	SER	L	123	-3.648	57.859	62.765	1.00	27.37	C
ATOM	4851	OG	SER	L	123	-3.335	56.701	62.003	1.00	24.63	O
ATOM	4852	N	ASP	L	124	-5.222	59.927	60.829	1.00	30.29	N
ATOM	4853	CA	ASP	L	124	-5.381	60.419	59.467	1.00	31.10	C
ATOM	4854	C	ASP	L	124	-4.416	59.704	58.549	1.00	31.06	C
ATOM	4855	O	ASP	L	124	-4.741	59.436	57.395	1.00	31.07	O
ATOM	4856	CB	ASP	L	124	-5.141	61.927	59.396	1.00	32.87	C
ATOM	4857	CG	ASP	L	124	-6.390	62.726	59.691	1.00	34.61	C
ATOM	4858	OD1	ASP	L	124	-7.349	62.599	58.902	1.00	34.85	O
ATOM	4859	OD2	ASP	L	124	-6.411	63.472	60.694	1.00	34.61	O
ATOM	4860	N	GLU	L	125	-3.232	59.404	59.073	1.00	30.87	N
ATOM	4861	CA	GLU	L	125	-2.198	58.692	58.337	1.00	31.89	C

FIG. 53-77

ATOM	4863	O	GLU	L	125	-2.379	56.786	56.868	1.00	32.57	O
ATOM	4864	CB	GLU	L	125	-0.927	58.622	59.182	1.00	31.97	C
ATOM	4865	CG	GLU	L	125	0.150	57.698	58.639	1.00	34.49	C
ATOM	4866	CD	GLU	L	125	1.429	57.742	59.454	1.00	35.13	C
ATOM	4867	OE1	GLU	L	125	1.416	58.245	60.604	1.00	35.50	O
ATOM	4868	OE2	GLU	L	125	2.465	57.269	58.940	1.00	35.88	O
ATOM	4869	N	GLN	L	126	-3.412	56.638	58.865	1.00	32.79	N
ATOM	4870	CA	GLN	L	126	-3.931	55.304	58.603	1.00	32.46	C
ATOM	4871	C	GLN	L	126	-5.097	55.409	57.619	1.00	33.57	C
ATOM	4872	O	GLN	L	126	-5.278	54.550	56.749	1.00	34.07	O
ATOM	4873	CB	GLN	L	126	-4.392	54.624	59.887	1.00	30.48	C
ATOM	4874	CG	GLN	L	126	-4.513	53.127	59.743	1.00	27.57	C
ATOM	4875	CD	GLN	L	126	-5.088	52.462	60.963	1.00	27.43	C
ATOM	4876	OE1	GLN	L	126	-6.161	52.828	61.438	1.00	25.65	O
ATOM	4877	NE2	GLN	L	126	-4.384	51.465	61.477	1.00	27.30	N
ATOM	4878	N	LEU	L	127	-5.879	56.473	57.748	1.00	34.76	N
ATOM	4879	CA	LEU	L	127	-7.001	56.700	56.848	1.00	36.08	C
ATOM	4880	C	LEU	L	127	-6.476	56.986	55.436	1.00	37.31	C
ATOM	4881	O	LEU	L	127	-7.070	56.554	54.442	1.00	36.78	O
ATOM	4882	CB	LEU	L	127	-7.859	57.870	57.345	1.00	36.18	C
ATOM	4883	CG	LEU	L	127	-9.224	57.533	57.961	1.00	36.61	C
ATOM	4884	CD1	LEU	L	127	-9.050	56.630	59.160	1.00	37.63	C
ATOM	4885	CD2	LEU	L	127	-9.963	58.812	58.348	1.00	35.88	C
ATOM	4886	N	LYS	L	128	-5.377	57.729	55.342	1.00	38.69	N
ATOM	4887	CA	LYS	L	128	-4.799	58.038	54.037	1.00	40.81	C
ATOM	4888	C	LYS	L	128	-4.191	56.746	53.497	1.00	41.40	C
ATOM	4889	O	LYS	L	128	-4.427	56.377	52.343	1.00	42.64	O
ATOM	4890	CB	LYS	L	128	-3.703	59.118	54.126	1.00	42.31	C
ATOM	4891	CG	LYS	L	128	-4.062	60.396	54.884	1.00	42.79	C
ATOM	4892	CD	LYS	L	128	-5.250	61.141	54.301	1.00	43.43	C
ATOM	4893	CE	LYS	L	128	-5.690	62.278	55.228	1.00	43.12	C
ATOM	4894	NZ	LYS	L	128	-6.313	61.792	56.503	1.00	41.82	N
ATOM	4895	N	SER	L	129	-3.459	56.037	54.361	1.00	40.89	N
ATOM	4896	CA	SER	L	129	-2.805	54.788	53.980	1.00	39.68	C
ATOM	4897	C	SER	L	129	-3.800	53.757	53.462	1.00	38.38	C
ATOM	4898	O	SER	L	129	-3.427	52.894	52.668	1.00	38.82	O
ATOM	4899	CB	SER	L	129	-1.978	54.210	55.137	1.00	40.35	C
ATOM	4900	OG	SER	L	129	-2.786	53.539	56.090	1.00	41.44	O
ATOM	4901	N	GLY	L	130	-5.044	53.816	53.943	1.00	36.60	N
ATOM	4902	CA	GLY	L	130	-6.058	52.894	53.455	1.00	34.28	C
ATOM	4903	C	GLY	L	130	-6.965	52.141	54.415	1.00	33.04	C
ATOM	4904	O	GLY	L	130	-7.991	51.603	53.983	1.00	32.64	O
ATOM	4905	N	THR	L	131	-6.631	52.100	55.700	1.00	31.29	N
ATOM	4906	CA	THR	L	131	-7.456	51.366	56.658	1.00	29.86	C
ATOM	4907	C	THR	L	131	-7.819	52.215	57.876	1.00	28.24	C
ATOM	4908	O	THR	L	131	-7.146	53.199	58.177	1.00	28.47	O
ATOM	4909	CB	THR	L	131	-6.749	50.056	57.102	1.00	30.36	C
ATOM	4910	OG1	THR	L	131	-6.373	49.301	55.944	1.00	32.17	O
ATOM	4911	CG2	THR	L	131	-7.670	49.191	57.942	1.00	31.50	C
ATOM	4912	N	ALA	L	132	-8.915	51.852	58.542	1.00	26.77	N
ATOM	4913	CA	ALA	L	132	-9.389	52.560	59.728	1.00	24.76	C
ATOM	4914	C	ALA	L	132	-9.377	51.630	60.943	1.00	22.96	C
ATOM	4915	O	ALA	L	132	-10.031	50.586	60.937	1.00	22.49	O
ATOM	4916	CB	ALA	L	132	-10.789	53.079	59.484	1.00	26.60	C
ATOM	4917	N	SER	L	133	-8.630	52.007	61.976	1.00	21.32	N
ATOM	4918	CA	SER	L	133	-8.522	51.200	63.187	1.00	19.59	C
ATOM	4919	C	SER	L	133	-8.748	52.028	64.444	1.00	18.17	C
ATOM	4920	O	SER	L	133	-7.912	52.856	64.819	1.00	17.68	O
ATOM	4921	CB	SER	L	133	-7.148	50.532	63.253	1.00	20.02	C
ATOM	4922	OG	SER	L	133	-6.865	49.830	62.053	1.00	20.61	O
ATOM	4923	N	VAL	L	134	-9.901	51.824	65.070	1.00	16.47	N
ATOM	4924	CA	VAL	L	134	-10.254	52.549	66.279	1.00	15.50	C
ATOM	4925	C	VAL	L	134	-9.679	51.711	67.417	1.00	15.65	C
ATOM	4926	O	VAL	L	134	-9.483	50.498	67.257	1.00	17.17	O
ATOM	4927	CB	VAL	L	134	-11.800	52.697	66.415	1.00	15.27	C
ATOM	4928	CG1	VAL	L	134	-12.149	53.794	67.418	1.00	11.88	C
ATOM	4929	CG2	VAL	L	134	-12.423	52.997	65.065	1.00	11.45	C
ATOM	4930	N	VAL	L	135	-9.383	52.343	68.548	1.00	13.24	N
ATOM	4931	CA	VAL	L	135	-8.792	51.633	69.668	1.00	11.67	C
ATOM	4932	C	VAL	L	135	9.208	52.078	70.984	1.00	12.59	C

FIG. 53-78

ATOM	4934	CB	VAL	L	135	-7.258	51.890	69.734	1.00	9.22	C
ATOM	4935	CG1	VAL	L	135	-6.637	51.171	70.913	1.00	7.65	C
ATOM	4936	CG2	VAL	L	135	-6.594	51.457	68.457	1.00	6.97	C
ATOM	4937	N	CYS	L	136	-9.693	51.127	71.861	1.00	11.53	N
ATOM	4938	CA	CYS	L	136	-10.219	51.471	73.165	1.00	11.78	C
ATOM	4939	C	CYS	L	136	-9.256	50.871	74.173	1.00	11.17	C
ATOM	4940	O	CYS	L	136	-8.738	49.769	73.957	1.00	10.47	O
ATOM	4941	CB	CYS	L	136	-11.619	50.925	73.374	1.00	13.27	C
ATOM	4942	SG	CYS	L	136	-12.448	51.737	74.772	1.00	16.80	S
ATOM	4943	N	LEU	L	137	-9.046	51.592	75.273	1.00	9.86	N
ATOM	4944	CA	LEU	L	137	-8.109	51.210	76.316	1.00	8.87	C
ATOM	4945	C	LEU	L	137	-8.717	51.281	77.712	1.00	9.05	C
ATOM	4946	O	LEU	L	137	-9.136	52.350	78.173	1.00	9.00	O
ATOM	4947	CB	LEU	L	137	-6.911	52.167	76.258	1.00	8.33	C
ATOM	4948	CG	LEU	L	137	-5.549	51.962	76.945	1.00	9.11	C
ATOM	4949	CD1	LEU	L	137	-4.769	53.275	76.806	1.00	6.19	C
ATOM	4950	CD2	LEU	L	137	-5.665	51.579	78.413	1.00	8.99	C
ATOM	4951	N	LEU	L	138	-8.737	50.142	78.393	1.00	8.04	N
ATOM	4952	CA	LEU	L	138	-9.232	50.068	79.754	1.00	7.27	C
ATOM	4953	C	LEU	L	138	-7.971	50.062	80.604	1.00	8.18	C
ATOM	4954	O	LEU	L	138	-7.334	49.024	80.787	1.00	9.08	O
ATOM	4955	CB	LEU	L	138	-10.005	48.768	79.976	1.00	8.15	C
ATOM	4956	CG	LEU	L	138	-11.401	48.604	79.373	1.00	6.72	C
ATOM	4957	CD1	LEU	L	138	-11.370	48.750	77.862	1.00	9.30	C
ATOM	4958	CD2	LEU	L	138	-11.918	47.243	79.753	1.00	7.37	C
ATOM	4959	N	ASN	L	139	-7.588	51.225	81.107	1.00	10.27	N
ATOM	4960	CA	ASN	L	139	-6.370	51.325	81.899	1.00	9.79	C
ATOM	4961	C	ASN	L	139	-6.509	50.941	83.353	1.00	8.49	C
ATOM	4962	O	ASN	L	139	-7.546	51.158	83.959	1.00	7.93	O
ATOM	4963	CB	ASN	L	139	-5.770	52.725	81.795	1.00	11.38	C
ATOM	4964	CG	ASN	L	139	-4.270	52.729	82.022	1.00	10.57	C
ATOM	4965	OD1	ASN	L	139	-3.524	52.111	81.271	1.00	10.47	O
ATOM	4966	ND2	ASN	L	139	-3.826	53.431	83.050	1.00	11.24	N
ATOM	4967	N	ASN	L	140	-5.436	50.361	83.885	1.00	9.18	N
ATOM	4968	CA	ASN	L	140	-5.316	49.910	85.278	1.00	8.78	C
ATOM	4969	C	ASN	L	140	-6.577	49.542	86.049	1.00	8.46	C
ATOM	4970	O	ASN	L	140	-7.055	50.321	86.885	1.00	7.23	O
ATOM	4971	CB	ASN	L	140	-4.478	50.897	86.097	1.00	10.31	C
ATOM	4972	CG	ASN	L	140	-3.059	51.042	85.564	1.00	13.49	C
ATOM	4973	OD1	ASN	L	140	-2.781	51.898	84.720	1.00	14.68	O
ATOM	4974	ND2	ASN	L	140	-2.155	50.207	86.055	1.00	16.04	N
ATOM	4975	N	PHE	L	141	-7.103	48.354	85.760	1.00	8.17	N
ATOM	4976	CA	PHE	L	141	-8.277	47.819	86.443	1.00	8.05	C
ATOM	4977	C	PHE	L	141	-7.827	46.507	87.077	1.00	10.50	C
ATOM	4978	O	PHE	L	141	-6.898	45.872	86.580	1.00	10.89	O
ATOM	4979	CB	PHE	L	141	-9.446	47.599	85.476	1.00	7.55	C
ATOM	4980	CG	PHE	L	141	-9.135	46.691	84.296	1.00	8.60	C
ATOM	4981	CD1	PHE	L	141	-8.330	47.126	83.254	1.00	9.02	C
ATOM	4982	CD2	PHE	L	141	-9.707	45.423	84.207	1.00	9.55	C
ATOM	4983	CE1	PHE	L	141	-8.092	46.313	82.138	1.00	11.26	C
ATOM	4984	CE2	PHE	L	141	-9.478	44.603	83.099	1.00	11.92	C
ATOM	4985	CZ	PHE	L	141	-8.671	45.045	82.062	1.00	12.77	C
ATOM	4986	N	TYR	L	142	-8.422	46.108	88.196	1.00	12.90	N
ATOM	4987	CA	TYR	L	142	-7.972	44.863	88.810	1.00	13.83	C
ATOM	4988	C	TYR	L	142	-8.500	43.532	88.249	1.00	16.80	C
ATOM	4989	O	TYR	L	142	-7.765	42.848	87.529	1.00	19.27	O
ATOM	4990	CB	TYR	L	142	-8.063	44.879	90.336	1.00	12.09	C
ATOM	4991	CG	TYR	L	142	-7.711	43.522	90.898	1.00	9.68	C
ATOM	4992	CD1	TYR	L	142	-6.610	42.815	90.405	1.00	7.12	C
ATOM	4993	CD2	TYR	L	142	-8.546	42.886	91.806	1.00	9.85	C
ATOM	4994	CE1	TYR	L	142	-6.360	41.514	90.788	1.00	6.75	C
ATOM	4995	CE2	TYR	L	142	-8.298	41.578	92.201	1.00	11.16	C
ATOM	4996	CZ	TYR	L	142	-7.207	40.896	91.682	1.00	7.17	C
ATOM	4997	OH	TYR	L	142	-6.957	39.612	92.076	1.00	5.07	O
ATOM	4998	N	PRO	L	143	-9.724	43.093	88.637	1.00	16.37	N
ATOM	4999	CA	PRO	L	143	-10.134	41.815	88.050	1.00	15.10	C
ATOM	5000	C	PRO	L	143	-9.923	41.889	86.557	1.00	15.25	C
ATOM	5001	O	PRO	L	143	-10.364	42.850	85.914	1.00	13.71	O
ATOM	5002	CB	PRO	L	143	-11.621	41.735	88.409	1.00	15.42	C
ATOM	5003	CG	PRO	L	143	-11.682	42.432	89.725	1.00	15.74	C

FIG. 53-79

ATOM	5005	N	ARG	L	144	-9.111	40.959	86.056	1.00	17.00	N
ATOM	5006	CA	ARG	L	144	-8.780	40.863	84.636	1.00	18.20	C
ATOM	5007	C	ARG	L	144	-10.097	40.758	83.876	1.00	19.31	C
ATOM	5008	O	ARG	L	144	-10.176	41.087	82.688	1.00	19.84	O
ATOM	5009	CB	ARG	L	144	-7.909	39.624	84.393	1.00	19.37	C
ATOM	5010	CG	ARG	L	144	-7.036	39.649	83.137	1.00	19.70	C
ATOM	5011	CD	ARG	L	144	-6.209	38.359	83.032	1.00	18.40	C
ATOM	5012	NE	ARG	L	144	-5.201	38.403	81.970	1.00	21.52	N
ATOM	5013	CZ	ARG	L	144	-3.895	38.179	82.149	1.00	21.68	C
ATOM	5014	NH1	ARG	L	144	-3.414	37.889	83.351	1.00	22.56	N
ATOM	5015	NH2	ARG	L	144	-3.063	38.229	81.118	1.00	22.06	N
ATOM	5016	N	GLU	L	145	-11.127	40.299	84.584	1.00	19.53	N
ATOM	5017	CA	GLU	L	145	-12.464	40.159	84.030	1.00	20.80	C
ATOM	5018	C	GLU	L	145	-13.128	41.510	83.690	1.00	21.40	C
ATOM	5019	O	GLU	L	145	-13.634	42.235	84.566	1.00	20.44	O
ATOM	5020	CB	GLU	L	145	-13.341	39.354	84.987	1.00	20.47	C
ATOM	5021	CG	GLU	L	145	-12.988	37.874	85.071	1.00	21.37	C
ATOM	5022	CD	GLU	L	145	-11.568	37.615	85.553	1.00	22.05	C
ATOM	5023	OE1	GLU	L	145	-11.310	37.693	86.773	1.00	21.03	O
ATOM	5024	OE2	GLU	L	145	-10.699	37.324	84.707	1.00	24.64	O
ATOM	5025	N	ALA	L	146	-13.101	41.843	82.407	1.00	21.20	N
ATOM	5026	CA	ALA	L	146	-13.701	43.066	81.913	1.00	21.63	C
ATOM	5027	C	ALA	L	146	-14.450	42.732	80.621	1.00	23.24	C
ATOM	5028	O	ALA	L	146	-14.173	41.717	79.974	1.00	23.86	O
ATOM	5029	CB	ALA	L	146	-12.624	44.096	81.653	1.00	20.72	C
ATOM	5030	N	LYS	L	147	-15.432	43.554	80.275	1.00	24.12	N
ATOM	5031	CA	LYS	L	147	-16.201	43.348	79.057	1.00	24.43	C
ATOM	5032	C	LYS	L	147	-15.997	44.575	78.183	1.00	25.90	C
ATOM	5033	O	LYS	L	147	-15.704	45.671	78.680	1.00	26.11	O
ATOM	5034	CB	LYS	L	147	-17.690	43.176	79.381	1.00	24.88	C
ATOM	5035	CG	LYS	L	147	-18.431	42.127	78.535	1.00	23.00	C
ATOM	5036	CD	LYS	L	147	-18.842	42.637	77.162	1.00	21.31	C
ATOM	5037	CE	LYS	L	147	-19.490	41.519	76.353	1.00	21.90	C
ATOM	5038	NZ	LYS	L	147	-19.871	41.911	74.964	1.00	19.83	N
ATOM	5039	N	VAL	L	148	-16.111	44.370	76.875	1.00	26.98	N
ATOM	5040	CA	VAL	L	148	-15.951	45.435	75.895	1.00	26.72	C
ATOM	5041	C	VAL	L	148	-17.060	45.253	74.865	1.00	27.07	C
ATOM	5042	O	VAL	L	148	-17.474	44.121	74.580	1.00	28.48	O
ATOM	5043	CB	VAL	L	148	-14.581	45.337	75.170	1.00	25.94	C
ATOM	5044	CG1	VAL	L	148	-14.311	46.595	74.394	1.00	24.38	C
ATOM	5045	CG2	VAL	L	148	-13.454	45.064	76.161	1.00	24.31	C
ATOM	5046	N	GLN	L	149	-17.588	46.360	74.361	1.00	26.55	N
ATOM	5047	CA	GLN	L	149	-18.646	46.322	73.355	1.00	26.89	C
ATOM	5048	C	GLN	L	149	-18.478	47.527	72.481	1.00	27.70	C
ATOM	5049	O	GLN	L	149	-18.187	48.614	72.974	1.00	28.41	O
ATOM	5050	CB	GLN	L	149	-20.025	46.377	73.996	1.00	26.69	C
ATOM	5051	CG	GLN	L	149	-20.756	45.070	73.958	1.00	27.95	C
ATOM	5052	CD	GLN	L	149	-21.890	45.024	74.947	1.00	30.34	C
ATOM	5053	OE1	GLN	L	149	-21.723	44.573	76.086	1.00	30.41	O
ATOM	5054	NE2	GLN	L	149	-23.056	45.471	74.520	1.00	31.39	N
ATOM	5055	N	TRP	L	150	-18.611	47.331	71.179	1.00	27.58	N
ATOM	5056	CA	TRP	L	150	-18.464	48.437	70.262	1.00	28.31	C
ATOM	5057	C	TRP	L	150	-19.781	48.759	69.587	1.00	31.55	C
ATOM	5058	O	TRP	L	150	-20.758	48.018	69.702	1.00	31.25	O
ATOM	5059	CB	TRP	L	150	-17.403	48.130	69.209	1.00	23.64	C
ATOM	5060	CG	TRP	L	150	-15.990	48.207	69.698	1.00	20.14	C
ATOM	5061	CD1	TRP	L	150	-15.239	47.185	70.207	1.00	19.18	C
ATOM	5062	CD2	TRP	L	150	-15.117	49.345	69.628	1.00	18.90	C
ATOM	5063	NE1	TRP	L	150	-13.953	47.609	70.441	1.00	17.86	N
ATOM	5064	CE2	TRP	L	150	-13.849	48.929	70.092	1.00	18.56	C
ATOM	5065	CE3	TRP	L	150	-15.281	50.675	69.214	1.00	16.93	C
ATOM	5066	CZ2	TRP	L	150	-12.753	49.798	70.154	1.00	17.58	C
ATOM	5067	CZ3	TRP	L	150	-14.194	51.535	69.277	1.00	15.09	C
ATOM	5068	CH2	TRP	L	150	-12.946	51.093	69.741	1.00	16.67	C
ATOM	5069	N	LYS	L	151	-19.795	49.894	68.900	1.00	36.22	N
ATOM	5070	CA	LYS	L	151	-20.952	50.362	68.159	1.00	39.51	C
ATOM	5071	C	LYS	L	151	-20.340	50.949	66.888	1.00	41.77	C
ATOM	5072	O	LYS	L	151	-19.170	51.349	66.876	1.00	42.22	O
ATOM	5073	CB	LYS	L	151	-21.690	51.470	68.927	1.00	39.92	C
ATOM	5074	CG	LYS	L	151	-21.854	51.230	70.426	1.00	43.00	C

FIG. 53-80

ATOM	5076	CE	LYS	L	151	-24.384	51.432	70.668	1.00	47.81	C
ATOM	5077	NZ	LYS	L	151	-24.367	52.720	71.438	1.00	49.14	N
ATOM	5078	N	VAL	L	152	-21.106	50.920	65.805	1.00	43.46	N
ATOM	5079	CA	VAL	L	152	-20.665	51.476	64.531	1.00	43.64	C
ATOM	5080	C	VAL	L	152	-21.553	52.672	64.207	1.00	43.81	C
ATOM	5081	O	VAL	L	152	-21.213	53.495	63.354	1.00	43.94	O
ATOM	5082	CB	VAL	L	152	-20.795	50.445	63.390	1.00	44.47	C
ATOM	5083	CG1	VAL	L	152	-22.265	50.156	63.094	1.00	44.41	C
ATOM	5084	CG2	VAL	L	152	-20.068	50.941	62.145	1.00	45.11	C
ATOM	5085	N	ASP	L	153	-22.713	52.700	64.865	1.00	43.39	N
ATOM	5086	CA	ASP	L	153	-23.741	53.732	64.733	1.00	44.01	C
ATOM	5087	C	ASP	L	153	-24.910	53.233	65.574	1.00	44.62	C
ATOM	5088	O	ASP	L	153	-26.004	52.977	65.066	1.00	45.88	O
ATOM	5089	CB	ASP	L	153	-24.200	53.889	63.278	1.00	44.29	C
ATOM	5090	CG	ASP	L	153	-23.754	55.197	62.657	1.00	44.59	C
ATOM	5091	OD1	ASP	L	153	-23.643	56.217	63.373	1.00	44.63	O
ATOM	5092	OD2	ASP	L	153	-23.506	55.200	61.434	1.00	46.20	O
ATOM	5093	N	ASN	L	154	-24.635	53.004	66.853	1.00	43.73	N
ATOM	5094	CA	ASN	L	154	-25.623	52.504	67.808	1.00	42.71	C
ATOM	5095	C	ASN	L	154	-25.945	51.014	67.643	1.00	41.97	C
ATOM	5096	O	ASN	L	154	-26.535	50.405	68.534	1.00	41.18	O
ATOM	5097	CB	ASN	L	154	-26.909	53.342	67.784	1.00	43.27	C
ATOM	5098	CG	ASN	L	154	-27.507	53.523	69.171	1.00	43.36	C
ATOM	5099	OD1	ASN	L	154	-26.791	53.492	70.182	1.00	44.42	O
ATOM	5100	ND2	ASN	L	154	-28.816	53.735	69.227	1.00	41.84	N
ATOM	5101	N	ALA	L	155	-25.540	50.426	66.518	1.00	41.02	N
ATOM	5102	CA	ALA	L	155	-25.758	48.999	66.271	1.00	39.62	C
ATOM	5103	C	ALA	L	155	-24.522	48.263	66.787	1.00	38.90	C
ATOM	5104	O	ALA	L	155	-23.401	48.768	66.660	1.00	38.99	O
ATOM	5105	CB	ALA	L	155	-25.954	48.740	64.789	1.00	38.88	C
ATOM	5106	N	LEU	L	156	-24.719	47.073	67.347	1.00	38.28	N
ATOM	5107	CA	LEU	L	156	-23.619	46.294	67.916	1.00	37.65	C
ATOM	5108	C	LEU	L	156	-22.635	45.673	66.933	1.00	37.26	C
ATOM	5109	O	LEU	L	156	-23.020	45.233	65.848	1.00	37.41	O
ATOM	5110	CB	LEU	L	156	-24.163	45.216	68.859	1.00	36.83	C
ATOM	5111	CG	LEU	L	156	-23.847	45.405	70.346	1.00	34.02	C
ATOM	5112	CD1	LEU	L	156	-22.342	45.392	70.532	1.00	33.39	C
ATOM	5113	CD2	LEU	L	156	-24.442	46.710	70.867	1.00	32.28	C
ATOM	5114	N	GLN	L	157	-21.362	45.642	67.325	1.00	37.11	N
ATOM	5115	CA	GLN	L	157	-20.303	45.064	66.495	1.00	36.71	C
ATOM	5116	C	GLN	L	157	-19.739	43.792	67.115	1.00	36.12	C
ATOM	5117	O	GLN	L	157	-19.786	43.620	68.335	1.00	34.66	O
ATOM	5118	CB	GLN	L	157	-19.168	46.063	66.262	1.00	36.57	C
ATOM	5119	CG	GLN	L	157	-19.523	47.200	65.322	1.00	37.72	C
ATOM	5120	CD	GLN	L	157	-20.160	46.716	64.032	1.00	38.91	C
ATOM	5121	OE1	GLN	L	157	-19.644	45.821	63.354	1.00	39.12	O
ATOM	5122	NE2	GLN	L	157	-21.312	47.279	63.707	1.00	39.65	N
ATOM	5123	N	SER	L	158	-19.215	42.913	66.262	1.00	36.33	N
ATOM	5124	CA	SER	L	158	-18.639	41.639	66.680	1.00	35.62	C
ATOM	5125	C	SER	L	158	-17.820	41.000	65.558	1.00	35.19	C
ATOM	5126	O	SER	L	158	-18.158	41.122	64.382	1.00	35.02	O
ATOM	5127	CB	SER	L	158	-19.753	40.680	67.101	1.00	35.10	C
ATOM	5128	OG	SER	L	158	-20.726	40.548	66.077	1.00	32.12	O
ATOM	5129	N	GLY	L	159	-16.727	40.338	65.927	1.00	34.60	N
ATOM	5130	CA	GLY	L	159	-15.888	39.674	64.941	1.00	33.06	C
ATOM	5131	C	GLY	L	159	-14.677	40.454	64.472	1.00	32.15	C
ATOM	5132	O	GLY	L	159	-13.600	39.896	64.287	1.00	33.10	O
ATOM	5133	N	ASN	L	160	-14.843	41.757	64.307	1.00	31.89	N
ATOM	5134	CA	ASN	L	160	-13.754	42.612	63.836	1.00	30.85	C
ATOM	5135	C	ASN	L	160	-12.910	43.226	64.953	1.00	30.84	C
ATOM	5136	O	ASN	L	160	-11.991	44.010	64.684	1.00	30.24	O
ATOM	5137	CB	ASN	L	160	-14.314	43.709	62.931	1.00	30.08	C
ATOM	5138	CG	ASN	L	160	-15.620	44.263	63.440	1.00	29.11	C
ATOM	5139	OD1	ASN	L	160	-15.864	44.285	64.648	1.00	28.52	O
ATOM	5140	ND2	ASN	L	160	-16.486	44.673	62.528	1.00	29.91	N
ATOM	5141	N	SER	L	161	-13.208	42.861	66.198	1.00	30.23	N
ATOM	5142	CA	SER	L	161	-12.471	43.383	67.346	1.00	29.43	C
ATOM	5143	C	SER	L	161	-11.579	42.338	68.021	1.00	28.71	C
ATOM	5144	O	SER	L	161	-11.992	41.191	68.218	1.00	28.95	O
ATOM	5145	CB	SER	L	161	-13.449	43.904	68.353	1.00	29.60	C

FIG. 53-81

ATOM	5147	N	GLN	L	162	-10.349	42.729	68.348	1.00	27.14	N
ATOM	5148	CA	GLN	L	162	-9.402	41.829	69.010	1.00	26.44	C
ATOM	5149	C	GLN	L	162	-8.672	42.481	70.187	1.00	26.49	C
ATOM	5150	O	GLN	L	162	-7.754	43.297	70.002	1.00	26.77	O
ATOM	5151	CB	GLN	L	162	-8.370	41.312	68.019	1.00	26.02	C
ATOM	5152	CG	GLN	L	162	-8.906	40.359	66.992	1.00	24.83	C
ATOM	5153	CD	GLN	L	162	-7.833	39.922	66.042	1.00	23.29	C
ATOM	5154	OE1	GLN	L	162	-7.586	40.574	65.031	1.00	24.66	O
ATOM	5155	NE2	GLN	L	162	-7.154	38.832	66.374	1.00	23.88	N
ATOM	5156	N	GLU	L	163	-9.057	42.095	71.397	1.00	24.82	N
ATOM	5157	CA	GLU	L	163	-8.436	42.650	72.583	1.00	23.67	C
ATOM	5158	C	GLU	L	163	-7.177	41.949	73.039	1.00	21.69	C
ATOM	5159	O	GLU	L	163	-6.864	40.835	72.615	1.00	21.45	O
ATOM	5160	CB	GLU	L	163	-9.436	42.747	73.729	1.00	25.41	C
ATOM	5161	CG	GLU	L	163	-10.291	41.535	73.934	1.00	29.25	C
ATOM	5162	CD	GLU	L	163	-11.719	41.914	74.253	1.00	33.17	C
ATOM	5163	OE1	GLU	L	163	-12.315	42.680	73.456	1.00	34.01	O
ATOM	5164	OE2	GLU	L	163	-12.238	41.454	75.299	1.00	35.13	O
ATOM	5165	N	SER	L	164	-6.444	42.636	73.900	1.00	19.82	N
ATOM	5166	CA	SER	L	164	-5.206	42.129	74.453	1.00	17.86	C
ATOM	5167	C	SER	L	164	-5.128	42.645	75.890	1.00	16.94	C
ATOM	5168	O	SER	L	164	-5.679	43.706	76.203	1.00	19.26	O
ATOM	5169	CB	SER	L	164	-4.033	42.647	73.619	1.00	16.64	C
ATOM	5170	OG	SER	L	164	-2.828	42.015	73.990	1.00	19.50	O
ATOM	5171	N	VAL	L	165	-4.505	41.875	76.772	1.00	14.24	N
ATOM	5172	CA	VAL	L	165	-4.359	42.260	78.168	1.00	11.37	C
ATOM	5173	C	VAL	L	165	-2.893	42.091	78.554	1.00	11.46	C
ATOM	5174	O	VAL	L	165	-2.204	41.218	78.020	1.00	11.36	O
ATOM	5175	CB	VAL	L	165	-5.243	41.383	79.078	1.00	9.55	C
ATOM	5176	CG1	VAL	L	165	-5.039	41.731	80.529	1.00	8.73	C
ATOM	5177	CG2	VAL	L	165	-6.693	41.574	78.723	1.00	11.84	C
ATOM	5178	N	THR	L	166	-2.401	42.955	79.435	1.00	10.28	N
ATOM	5179	CA	THR	L	166	-1.016	42.874	79.878	1.00	10.52	C
ATOM	5180	C	THR	L	166	-0.858	41.859	81.020	1.00	12.19	C
ATOM	5181	O	THR	L	166	-1.836	41.311	81.533	1.00	11.21	O
ATOM	5182	CB	THR	L	166	-0.516	44.252	80.386	1.00	9.47	C
ATOM	5183	OG1	THR	L	166	-1.354	44.696	81.460	1.00	9.54	O
ATOM	5184	CG2	THR	L	166	-0.545	45.298	79.277	1.00	5.19	C
ATOM	5185	N	GLU	L	167	0.383	41.534	81.351	1.00	14.91	N
ATOM	5186	CA	GLU	L	167	0.645	40.645	82.473	1.00	17.53	C
ATOM	5187	C	GLU	L	167	0.467	41.569	83.691	1.00	18.96	C
ATOM	5188	O	GLU	L	167	0.747	42.766	83.603	1.00	20.99	O
ATOM	5189	CB	GLU	L	167	2.079	40.104	82.413	1.00	19.23	C
ATOM	5190	CG	GLU	L	167	2.337	39.039	81.343	1.00	22.37	C
ATOM	5191	CD	GLU	L	167	1.759	37.676	81.701	1.00	25.92	C
ATOM	5192	OE1	GLU	L	167	1.837	37.279	82.888	1.00	27.11	O
ATOM	5193	OE2	GLU	L	167	1.223	37.000	80.792	1.00	26.04	O
ATOM	5194	N	GLN	L	168	0.004	41.032	84.812	1.00	19.68	N
ATOM	5195	CA	GLN	L	168	-0.225	41.832	86.016	1.00	20.51	C
ATOM	5196	C	GLN	L	168	0.942	42.751	86.355	1.00	21.66	C
ATOM	5197	O	GLN	L	168	2.096	42.322	86.312	1.00	21.63	O
ATOM	5198	CB	GLN	L	168	-0.517	40.910	87.197	1.00	21.14	C
ATOM	5199	CG	GLN	L	168	-0.921	41.622	88.455	1.00	19.06	C
ATOM	5200	CD	GLN	L	168	-1.487	40.680	89.478	1.00	18.83	C
ATOM	5201	OE1	GLN	L	168	-0.861	39.681	89.841	1.00	17.90	O
ATOM	5202	NE2	GLN	L	168	-2.676	40.993	89.963	1.00	20.30	N
ATOM	5203	N	ASP	L	169	0.635	44.003	86.709	1.00	22.03	N
ATOM	5204	CA	ASP	L	169	1.682	44.972	87.033	1.00	22.10	C
ATOM	5205	C	ASP	L	169	2.379	44.710	88.359	1.00	21.82	C
ATOM	5206	O	ASP	L	169	1.735	44.432	89.378	1.00	21.33	O
ATOM	5207	CB	ASP	L	169	1.171	46.413	86.978	1.00	23.06	C
ATOM	5208	CG	ASP	L	169	2.313	47.422	86.896	1.00	24.41	C
ATOM	5209	OD1	ASP	L	169	2.862	47.788	87.953	1.00	27.41	O
ATOM	5210	OD2	ASP	L	169	2.716	47.804	85.776	1.00	22.98	O
ATOM	5211	N	SER	L	170	3.703	44.840	88.329	1.00	22.45	N
ATOM	5212	CA	SER	L	170	4.577	44.593	89.479	1.00	21.46	C
ATOM	5213	C	SER	L	170	4.449	45.585	90.616	1.00	19.16	C
ATOM	5214	O	SER	L	170	4.692	45.240	91.768	1.00	18.27	O
ATOM	5215	CB	SER	L	170	6.037	44.511	89.022	1.00	22.76	C

FIG. 53-82

ATOM	5218	CA	LYS	L	171	3.909	47.851	91.299	1.00	17.00	C
ATOM	5219	C	LYS	L	171	2.500	47.878	91.900	1.00	15.97	C
ATOM	5220	O	LYS	L	171	2.346	47.774	93.117	1.00	16.17	O
ATOM	5221	CB	LYS	L	171	4.248	49.231	90.722	1.00	17.18	C
ATOM	5222	CG	LYS	L	171	5.715	49.675	90.880	1.00	16.28	C
ATOM	5223	CD	LYS	L	171	6.701	48.884	90.022	1.00	16.75	C
ATOM	5224	CE	LYS	L	171	6.455	49.058	88.521	1.00	17.21	C
ATOM	5225	NZ	LYS	L	171	6.605	50.459	88.042	1.00	15.68	N
ATOM	5226	N	ASP	L	172	1.475	47.934	91.052	1.00	14.88	N
ATOM	5227	CA	ASP	L	172	0.101	48.028	91.542	1.00	15.20	C
ATOM	5228	C	ASP	L	172	-0.899	46.867	91.448	1.00	13.21	C
ATOM	5229	O	ASP	L	172	-2.074	47.033	91.801	1.00	11.47	O
ATOM	5230	CB	ASP	L	172	-0.544	49.330	91.032	1.00	20.61	C
ATOM	5231	CG	ASP	L	172	-0.329	49.581	89.533	1.00	24.63	C
ATOM	5232	OD1	ASP	L	172	0.829	49.697	89.086	1.00	26.58	O
ATOM	5233	OD2	ASP	L	172	-1.334	49.726	88.807	1.00	28.09	O
ATOM	5234	N	SER	L	173	-0.453	45.703	90.983	1.00	11.82	N
ATOM	5235	CA	SER	L	173	-1.313	44.520	90.875	1.00	9.20	C
ATOM	5236	C	SER	L	173	-2.608	44.676	90.071	1.00	9.25	C
ATOM	5237	O	SER	L	173	-3.592	43.976	90.323	1.00	11.51	O
ATOM	5238	CB	SER	L	173	-1.648	43.968	92.260	1.00	7.54	C
ATOM	5239	OG	SER	L	173	-0.472	43.679	92.991	1.00	4.68	O
ATOM	5240	N	THR	L	174	-2.600	45.570	89.093	1.00	7.82	N
ATOM	5241	CA	THR	L	174	-3.758	45.794	88.242	1.00	7.08	C
ATOM	5242	C	THR	L	174	-3.377	45.282	86.867	1.00	6.59	C
ATOM	5243	O	THR	L	174	-2.269	44.775	86.696	1.00	7.57	O
ATOM	5244	CB	THR	L	174	-4.112	47.289	88.155	1.00	8.05	C
ATOM	5245	OG1	THR	L	174	-2.999	48.019	87.622	1.00	6.17	O
ATOM	5246	CG2	THR	L	174	-4.459	47.833	89.533	1.00	7.23	C
ATOM	5247	N	TYR	L	175	-4.294	45.385	85.909	1.00	6.94	N
ATOM	5248	CA	TYR	L	175	-4.075	44.947	84.522	1.00	9.29	C
ATOM	5249	C	TYR	L	175	-4.596	46.049	83.608	1.00	9.75	C
ATOM	5250	O	TYR	L	175	-5.155	47.039	84.071	1.00	9.70	O
ATOM	5251	CB	TYR	L	175	-4.906	43.694	84.199	1.00	10.57	C
ATOM	5252	CG	TYR	L	175	-4.476	42.417	84.857	1.00	11.63	C
ATOM	5253	CD1	TYR	L	175	-3.547	41.589	84.249	1.00	12.07	C
ATOM	5254	CD2	TYR	L	175	-5.007	42.025	86.087	1.00	15.20	C
ATOM	5255	CE1	TYR	L	175	-3.152	40.404	84.841	1.00	13.77	C
ATOM	5256	CE2	TYR	L	175	-4.614	40.831	86.693	1.00	14.73	C
ATOM	5257	CZ	TYR	L	175	-3.688	40.030	86.057	1.00	14.27	C
ATOM	5258	OH	TYR	L	175	-3.301	38.844	86.619	1.00	18.68	O
ATOM	5259	N	SER	L	176	-4.462	45.852	82.306	1.00	11.16	N
ATOM	5260	CA	SER	L	176	-4.985	46.803	81.337	1.00	11.52	C
ATOM	5261	C	SER	L	176	-5.392	46.037	80.090	1.00	12.38	C
ATOM	5262	O	SER	L	176	-4.954	44.910	79.886	1.00	11.64	O
ATOM	5263	CB	SER	L	176	-3.969	47.890	81.036	1.00	11.51	C
ATOM	5264	OG	SER	L	176	-3.744	48.662	82.210	1.00	14.01	O
ATOM	5265	N	LEU	L	177	-6.274	46.611	79.284	1.00	16.50	N
ATOM	5266	CA	LEU	L	177	-6.749	45.928	78.075	1.00	18.46	C
ATOM	5267	C	LEU	L	177	-6.842	46.873	76.893	1.00	18.55	C
ATOM	5268	O	LEU	L	177	-7.090	48.069	77.063	1.00	19.01	O
ATOM	5269	CB	LEU	L	177	-8.126	45.291	78.342	1.00	19.24	C
ATOM	5270	CG	LEU	L	177	-8.809	44.351	77.334	1.00	19.52	C
ATOM	5271	CD1	LEU	L	177	-9.779	43.441	78.058	1.00	16.66	C
ATOM	5272	CD2	LEU	L	177	-9.528	45.125	76.248	1.00	19.49	C
ATOM	5273	N	SER	L	178	-6.616	46.348	75.699	1.00	18.94	N
ATOM	5274	CA	SER	L	178	-6.713	47.173	74.508	1.00	20.49	C
ATOM	5275	C	SER	L	178	-7.591	46.468	73.495	1.00	20.65	C
ATOM	5276	O	SER	L	178	-7.305	45.332	73.099	1.00	19.96	O
ATOM	5277	CB	SER	L	178	-5.337	47.463	73.906	1.00	21.19	C
ATOM	5278	OG	SER	L	178	-4.732	46.293	73.384	1.00	23.79	O
ATOM	5279	N	SER	L	179	-8.708	47.101	73.150	1.00	20.87	N
ATOM	5280	CA	SER	L	179	-9.613	46.528	72.179	1.00	20.29	C
ATOM	5281	C	SER	L	179	-9.659	47.394	70.938	1.00	19.00	C
ATOM	5282	O	SER	L	179	-10.183	48.502	70.965	1.00	20.70	O
ATOM	5283	CB	SER	L	179	-11.011	46.344	72.757	1.00	20.27	C
ATOM	5284	OG	SER	L	179	-11.775	45.498	71.908	1.00	23.08	O
ATOM	5285	N	THR	L	180	-9.062	46.883	69.869	1.00	16.84	N
ATOM	5286	CA	THR	L	180	-9.000	47.541	68.570	1.00	14.41	C
ATOM	5287	C	THR	L	180	-10.151	47.047	67.694	1.00	15.07	C

FIG. 53-83

ATOM	5289	CB	THR	L	180	-7.708	47.142	67.872	1.00	10.71	C
ATOM	5290	OG1	THR	L	180	-6.640	47.187	68.822	1.00	6.75	O
ATOM	5291	CG2	THR	L	180	-7.404	48.071	66.701	1.00	9.72	C
ATOM	5292	N	LEU	L	181	-10.787	47.966	66.956	1.00	13.84	N
ATOM	5293	CA	LEU	L	181	-11.886	47.610	66.051	1.00	12.92	C
ATOM	5294	C	LEU	L	181	-11.428	47.989	64.666	1.00	12.23	C
ATOM	5295	O	LEU	L	181	-11.007	49.109	64.460	1.00	13.31	O
ATOM	5296	CB	LEU	L	181	-13.173	48.369	66.377	1.00	12.17	C
ATOM	5297	CG	LEU	L	181	-14.419	47.790	65.692	1.00	13.24	C
ATOM	5298	CD1	LEU	L	181	-14.774	46.483	66.366	1.00	14.73	C
ATOM	5299	CD2	LEU	L	181	-15.603	48.732	65.753	1.00	10.88	C
ATOM	5300	N	THR	L	182	-11.523	47.074	63.710	1.00	14.78	N
ATOM	5301	CA	THR	L	182	-11.065	47.377	62.362	1.00	17.68	C
ATOM	5302	C	THR	L	182	-12.143	47.375	61.277	1.00	20.12	C
ATOM	5303	O	THR	L	182	-13.009	46.486	61.221	1.00	20.43	O
ATOM	5304	CB	THR	L	182	-9.922	46.434	61.929	1.00	17.07	C
ATOM	5305	OG1	THR	L	182	-9.398	45.753	63.078	1.00	19.00	O
ATOM	5306	CG2	THR	L	182	-8.799	47.237	61.279	1.00	15.70	C
ATOM	5307	N	LEU	L	183	-12.082	48.401	60.433	1.00	19.48	N
ATOM	5308	CA	LEU	L	183	-12.994	48.570	59.315	1.00	20.51	C
ATOM	5309	C	LEU	L	183	-12.102	49.119	58.208	1.00	21.81	C
ATOM	5310	O	LEU	L	183	-11.075	49.747	58.489	1.00	22.53	O
ATOM	5311	CB	LEU	L	183	-14.074	49.617	59.626	1.00	21.14	C
ATOM	5312	CG	LEU	L	183	-14.678	49.864	61.016	1.00	22.09	C
ATOM	5313	CD1	LEU	L	183	-13.813	50.846	61.819	1.00	21.67	C
ATOM	5314	CD2	LEU	L	183	-16.069	50.460	60.835	1.00	22.48	C
ATOM	5315	N	SER	L	184	-12.450	48.865	56.952	1.00	23.13	N
ATOM	5316	CA	SER	L	184	-11.647	49.403	55.859	1.00	24.35	C
ATOM	5317	C	SER	L	184	-11.875	50.911	55.867	1.00	25.23	C
ATOM	5318	O	SER	L	184	-12.862	51.383	56.441	1.00	23.92	O
ATOM	5319	CB	SER	L	184	-12.076	48.811	54.507	1.00	23.84	C
ATOM	5320	OG	SER	L	184	-13.421	49.132	54.177	1.00	22.29	O
ATOM	5321	N	LYS	L	185	-10.960	51.664	55.262	1.00	27.81	N
ATOM	5322	CA	LYS	L	185	-11.097	53.121	55.176	1.00	29.86	C
ATOM	5323	C	LYS	L	185	-12.488	53.424	54.636	1.00	30.28	C
ATOM	5324	O	LYS	L	185	-13.128	54.395	55.034	1.00	29.66	O
ATOM	5325	CB	LYS	L	185	-10.063	53.688	54.201	1.00	31.37	C
ATOM	5326	CG	LYS	L	185	-10.308	55.121	53.777	1.00	32.79	C
ATOM	5327	CD	LYS	L	185	-9.946	56.088	54.873	1.00	34.93	C
ATOM	5328	CE	LYS	L	185	-10.021	57.528	54.374	1.00	37.29	C
ATOM	5329	NZ	LYS	L	185	-9.371	57.706	53.053	1.00	38.05	N
ATOM	5330	N	ALA	L	186	-12.941	52.562	53.730	1.00	30.68	N
ATOM	5331	CA	ALA	L	186	-14.247	52.697	53.123	1.00	30.54	C
ATOM	5332	C	ALA	L	186	-15.360	52.612	54.175	1.00	30.37	C
ATOM	5333	O	ALA	L	186	-15.930	53.637	54.540	1.00	29.84	O
ATOM	5334	CB	ALA	L	186	-14.425	51.644	52.045	1.00	31.15	C
ATOM	5335	N	ASP	L	187	-15.604	51.425	54.730	1.00	30.03	N
ATOM	5336	CA	ASP	L	187	-16.672	51.269	55.722	1.00	30.35	C
ATOM	5337	C	ASP	L	187	-16.644	52.238	56.895	1.00	29.09	C
ATOM	5338	O	ASP	L	187	-17.659	52.427	57.563	1.00	28.33	O
ATOM	5339	CB	ASP	L	187	-16.791	49.834	56.245	1.00	32.83	C
ATOM	5340	CG	ASP	L	187	-18.020	49.646	57.136	1.00	35.98	C
ATOM	5341	OD1	ASP	L	187	-19.134	50.044	56.714	1.00	37.38	O
ATOM	5342	OD2	ASP	L	187	-17.872	49.139	58.273	1.00	37.57	O
ATOM	5343	N	TYR	L	188	-15.487	52.832	57.172	1.00	28.85	N
ATOM	5344	CA	TYR	L	188	-15.403	53.804	58.257	1.00	28.55	C
ATOM	5345	C	TYR	L	188	-16.148	55.027	57.750	1.00	29.22	C
ATOM	5346	O	TYR	L	188	-17.145	55.456	58.338	1.00	28.87	O
ATOM	5347	CB	TYR	L	188	-13.952	54.171	58.562	1.00	26.77	C
ATOM	5348	CG	TYR	L	188	-13.789	54.987	59.819	1.00	23.61	C
ATOM	5349	CD1	TYR	L	188	-13.874	54.388	61.074	1.00	23.89	C
ATOM	5350	CD2	TYR	L	188	-13.541	56.351	59.760	1.00	24.55	C
ATOM	5351	CE1	TYR	L	188	-13.718	55.131	62.242	1.00	22.87	C
ATOM	5352	CE2	TYR	L	188	-13.379	57.109	60.925	1.00	23.85	C
ATOM	5353	CZ	TYR	L	188	-13.469	56.492	62.161	1.00	24.60	C
ATOM	5354	OH	TYR	L	188	-13.294	57.221	63.314	1.00	25.17	O
ATOM	5355	N	GLU	L	189	-15.679	55.551	56.621	1.00	30.25	N
ATOM	5356	CA	GLU	L	189	-16.294	56.709	55.989	1.00	31.78	C
ATOM	5357	C	GLU	L	189	-17.635	56.234	55.427	1.00	32.83	C
ATOM	5358	O	GLU	L	189	-17.751	55.861	54.253	1.00	33.41	O

FIG. 53-84

ATOM	5360	CG	GLU	L	189	-14.039	57.792	55.365	1.00	35.25	C
ATOM	5361	CD	GLU	L	189	-13.155	58.303	54.227	1.00	38.13	C
ATOM	5362	OE1	GLU	L	189	-12.850	57.522	53.286	1.00	38.01	O
ATOM	5363	OE2	GLU	L	189	-12.735	59.482	54.280	1.00	37.07	O
ATOM	5364	N	LYS	L	190	-18.629	56.202	56.308	1.00	33.88	N
ATOM	5365	CA	LYS	L	190	-19.982	55.765	55.984	1.00	35.62	C
ATOM	5366	C	LYS	L	190	-20.819	55.887	57.240	1.00	36.04	C
ATOM	5367	O	LYS	L	190	-22.023	56.113	57.180	1.00	35.82	O
ATOM	5368	CB	LYS	L	190	-19.988	54.298	55.552	1.00	37.09	C
ATOM	5369	CG	LYS	L	190	-21.375	53.697	55.331	1.00	39.08	C
ATOM	5370	CD	LYS	L	190	-21.263	52.280	54.793	1.00	39.92	C
ATOM	5371	CE	LYS	L	190	-22.619	51.693	54.452	1.00	40.51	C
ATOM	5372	NZ	LYS	L	190	-23.432	51.415	55.662	1.00	41.41	N
ATOM	5373	N	HIS	L	191	-20.175	55.696	58.382	1.00	36.86	N
ATOM	5374	CA	HIS	L	191	-20.867	55.765	59.651	1.00	38.35	C
ATOM	5375	C	HIS	L	191	-20.559	57.060	60.375	1.00	38.02	C
ATOM	5376	O	HIS	L	191	-19.904	57.946	59.811	1.00	38.09	O
ATOM	5377	CB	HIS	L	191	-20.515	54.547	60.496	1.00	41.04	C
ATOM	5378	CG	HIS	L	191	-20.845	53.250	59.827	1.00	43.74	C
ATOM	5379	ND1	HIS	L	191	-21.990	52.534	60.109	1.00	45.64	N
ATOM	5380	CD2	HIS	L	191	-20.188	52.546	58.876	1.00	44.80	C
ATOM	5381	CE1	HIS	L	191	-22.019	51.443	59.364	1.00	46.20	C
ATOM	5382	NE2	HIS	L	191	-20.936	51.428	58.605	1.00	46.13	N
ATOM	5383	N	LYS	L	192	-21.049	57.180	61.606	1.00	37.21	N
ATOM	5384	CA	LYS	L	192	-20.834	58.391	62.379	1.00	35.55	C
ATOM	5385	C	LYS	L	192	-20.311	58.150	63.784	1.00	34.21	C
ATOM	5386	O	LYS	L	192	-19.176	58.517	64.080	1.00	33.55	O
ATOM	5387	CB	LYS	L	192	-22.129	59.206	62.453	1.00	36.25	C
ATOM	5388	CG	LYS	L	192	-21.924	60.697	62.642	1.00	36.77	C
ATOM	5389	CD	LYS	L	192	-21.449	61.346	61.354	1.00	38.24	C
ATOM	5390	CE	LYS	L	192	-21.185	62.828	61.534	1.00	38.31	C
ATOM	5391	NZ	LYS	L	192	-20.072	63.050	62.495	1.00	39.59	N
ATOM	5392	N	VAL	L	193	-21.130	57.540	64.643	1.00	33.66	N
ATOM	5393	CA	VAL	L	193	-20.753	57.306	66.042	1.00	33.51	C
ATOM	5394	C	VAL	L	193	-20.094	55.977	66.405	1.00	32.45	C
ATOM	5395	O	VAL	L	193	-20.729	54.917	66.369	1.00	33.05	O
ATOM	5396	CB	VAL	L	193	-21.947	57.577	67.014	1.00	34.88	C
ATOM	5397	CG1	VAL	L	193	-23.222	56.937	66.500	1.00	36.25	C
ATOM	5398	CG2	VAL	L	193	-21.632	57.050	68.406	1.00	34.56	C
ATOM	5399	N	TYR	L	194	-18.837	56.066	66.837	1.00	30.50	N
ATOM	5400	CA	TYR	L	194	-18.056	54.906	67.239	1.00	29.68	C
ATOM	5401	C	TYR	L	194	-17.936	54.879	68.756	1.00	28.79	C
ATOM	5402	O	TYR	L	194	-17.132	55.612	69.340	1.00	28.23	O
ATOM	5403	CB	TYR	L	194	-16.677	54.952	66.585	1.00	30.77	C
ATOM	5404	CG	TYR	L	194	-16.752	54.849	65.082	1.00	31.80	C
ATOM	5405	CD1	TYR	L	194	-16.927	53.614	64.460	1.00	33.05	C
ATOM	5406	CD2	TYR	L	194	-16.710	55.990	64.283	1.00	32.55	C
ATOM	5407	CE1	TYR	L	194	-17.066	53.517	63.076	1.00	34.52	C
ATOM	5408	CE2	TYR	L	194	-16.847	55.906	62.901	1.00	33.29	C
ATOM	5409	CZ	TYR	L	194	-17.026	54.667	62.303	1.00	34.31	C
ATOM	5410	OH	TYR	L	194	-17.166	54.567	60.939	1.00	35.51	O
ATOM	5411	N	ALA	L	195	-18.738	54.024	69.387	1.00	28.06	N
ATOM	5412	CA	ALA	L	195	-18.762	53.909	70.844	1.00	26.33	C
ATOM	5413	C	ALA	L	195	-18.081	52.676	71.419	1.00	24.97	C
ATOM	5414	O	ALA	L	195	-18.228	51.566	70.916	1.00	23.70	O
ATOM	5415	CB	ALA	L	195	-20.195	53.984	71.349	1.00	26.18	C
ATOM	5416	N	CYS	L	196	-17.356	52.900	72.507	1.00	24.91	N
ATOM	5417	CA	CYS	L	196	-16.644	51.857	73.230	1.00	23.12	C
ATOM	5418	C	CYS	L	196	-17.325	51.725	74.582	1.00	22.46	C
ATOM	5419	O	CYS	L	196	-17.170	52.594	75.432	1.00	21.59	O
ATOM	5420	CB	CYS	L	196	-15.177	52.259	73.437	1.00	21.41	C
ATOM	5421	SG	CYS	L	196	-14.373	51.154	74.618	1.00	22.26	S
ATOM	5422	N	GLU	L	197	-18.143	50.692	74.743	1.00	24.50	N
ATOM	5423	CA	GLU	L	197	-18.865	50.443	75.993	1.00	26.84	C
ATOM	5424	C	GLU	L	197	-18.065	49.467	76.837	1.00	26.75	C
ATOM	5425	O	GLU	L	197	-17.591	48.453	76.325	1.00	26.00	O
ATOM	5426	CB	GLU	L	197	-20.259	49.861	75.707	1.00	29.41	C
ATOM	5427	CG	GLU	L	197	-21.032	49.408	76.951	1.00	32.09	C
ATOM	5428	CD	GLU	L	197	-22.365	48.731	76.627	1.00	35.08	C
ATOM	5429	OE1	GLU	L	197	-22.526	48.226	75.492	1.00	33.57	O

FIG. 53-85

ATOM	5431	N	VAL	L	198	-17.925	49.775	78.125	1.00	27.83	N
ATOM	5432	CA	VAL	L	198	-17.165	48.936	79.048	1.00	28.59	C
ATOM	5433	C	VAL	L	198	-17.918	48.592	80.336	1.00	28.86	C
ATOM	5434	O	VAL	L	198	-18.672	49.413	80.864	1.00	28.87	O
ATOM	5435	CB	VAL	L	198	-15.834	49.610	79.441	1.00	29.04	C
ATOM	5436	CG1	VAL	L	198	-15.016	48.672	80.323	1.00	30.38	C
ATOM	5437	CG2	VAL	L	198	-15.046	50.012	78.192	1.00	27.67	C
ATOM	5438	N	THR	L	199	-17.681	47.386	80.850	1.00	29.52	N
ATOM	5439	CA	THR	L	199	-18.316	46.906	82.080	1.00	29.04	C
ATOM	5440	C	THR	L	199	-17.256	46.289	83.013	1.00	29.21	C
ATOM	5441	O	THR	L	199	-16.282	45.691	82.547	1.00	29.24	O
ATOM	5442	CB	THR	L	199	-19.381	45.852	81.759	1.00	28.14	C
ATOM	5443	OG1	THR	L	199	-20.075	46.226	80.562	1.00	25.12	O
ATOM	5444	CG2	THR	L	199	-20.374	45.750	82.894	1.00	27.36	C
ATOM	5445	N	HIS	L	200	-17.459	46.400	84.323	1.00	28.56	N
ATOM	5446	CA	HIS	L	200	-16.486	45.884	85.291	1.00	28.22	C
ATOM	5447	C	HIS	L	200	-17.031	46.131	86.697	1.00	29.26	C
ATOM	5448	O	HIS	L	200	-18.082	46.755	86.845	1.00	30.25	O
ATOM	5449	CB	HIS	L	200	-15.165	46.659	85.114	1.00	26.36	C
ATOM	5450	CG	HIS	L	200	-14.007	46.097	85.878	1.00	24.47	C
ATOM	5451	ND1	HIS	L	200	-13.423	46.756	86.936	1.00	25.60	N
ATOM	5452	CD2	HIS	L	200	-13.296	44.958	85.711	1.00	24.69	C
ATOM	5453	CE1	HIS	L	200	-12.404	46.052	87.386	1.00	24.64	C
ATOM	5454	NE2	HIS	L	200	-12.304	44.955	86.659	1.00	24.23	N
ATOM	5455	N	GLN	L	201	-16.382	45.568	87.718	1.00	30.03	N
ATOM	5456	CA	GLN	L	201	-16.793	45.834	89.102	1.00	31.30	C
ATOM	5457	C	GLN	L	201	-16.113	47.175	89.326	1.00	30.74	C
ATOM	5458	O	GLN	L	201	-15.063	47.435	88.734	1.00	31.30	O
ATOM	5459	CB	GLN	L	201	-16.189	44.837	90.098	1.00	32.87	C
ATOM	5460	CG	GLN	L	201	-16.631	43.395	89.984	1.00	36.94	C
ATOM	5461	CD	GLN	L	201	-16.046	42.536	91.100	1.00	39.17	C
ATOM	5462	OE1	GLN	L	201	-15.413	41.511	90.850	1.00	42.29	O
ATOM	5463	NE2	GLN	L	201	-16.245	42.964	92.336	1.00	38.36	N
ATOM	5464	N	GLY	L	202	-16.673	48.027	90.168	1.00	30.22	N
ATOM	5465	CA	GLY	L	202	-16.042	49.318	90.386	1.00	28.92	C
ATOM	5466	C	GLY	L	202	-16.707	50.315	89.463	1.00	27.74	C
ATOM	5467	O	GLY	L	202	-17.014	51.434	89.877	1.00	27.84	O
ATOM	5468	N	LEU	L	203	-16.879	49.928	88.200	1.00	26.12	N
ATOM	5469	CA	LEU	L	203	-17.573	50.770	87.239	1.00	25.22	C
ATOM	5470	C	LEU	L	203	-19.024	50.467	87.547	1.00	26.14	C
ATOM	5471	O	LEU	L	203	-19.561	49.448	87.111	1.00	27.79	O
ATOM	5472	CB	LEU	L	203	-17.263	50.379	85.789	1.00	22.88	C
ATOM	5473	CG	LEU	L	203	-15.948	50.884	85.186	1.00	22.14	C
ATOM	5474	CD1	LEU	L	203	-15.916	50.610	83.697	1.00	20.58	C
ATOM	5475	CD2	LEU	L	203	-15.794	52.371	85.446	1.00	22.72	C
ATOM	5476	N	SER	L	204	-19.600	51.299	88.404	1.00	26.56	N
ATOM	5477	CA	SER	L	204	-20.985	51.187	88.853	1.00	26.25	C
ATOM	5478	C	SER	L	204	-21.965	50.924	87.700	1.00	27.59	C
ATOM	5479	O	SER	L	204	-22.775	49.987	87.750	1.00	28.27	O
ATOM	5480	CB	SER	L	204	-21.355	52.472	89.599	1.00	25.01	C
ATOM	5481	OG	SER	L	204	-20.257	53.382	89.615	1.00	18.30	O
ATOM	5482	N	SER	L	205	-21.880	51.759	86.668	1.00	27.10	N
ATOM	5483	CA	SER	L	205	-22.721	51.638	85.486	1.00	26.02	C
ATOM	5484	C	SER	L	205	-21.739	51.597	84.310	1.00	26.45	C
ATOM	5485	O	SER	L	205	-20.614	52.096	84.418	1.00	27.30	O
ATOM	5486	CB	SER	L	205	-23.647	52.858	85.362	1.00	25.69	C
ATOM	5487	OG	SER	L	205	-24.017	53.391	86.631	1.00	24.11	O
ATOM	5488	N	PRO	L	206	-22.132	50.972	83.189	1.00	25.99	N
ATOM	5489	CA	PRO	L	206	-21.263	50.877	82.011	1.00	25.85	C
ATOM	5490	C	PRO	L	206	-20.719	52.224	81.541	1.00	25.60	C
ATOM	5491	O	PRO	L	206	-21.465	53.202	81.430	1.00	25.34	O
ATOM	5492	CB	PRO	L	206	-22.183	50.243	80.969	1.00	25.19	C
ATOM	5493	CG	PRO	L	206	-23.020	49.324	81.803	1.00	25.62	C
ATOM	5494	CD	PRO	L	206	-23.375	50.208	82.981	1.00	26.67	C
ATOM	5495	N	VAL	L	207	-19.413	52.267	81.286	1.00	25.53	N
ATOM	5496	CA	VAL	L	207	-18.744	53.479	80.821	1.00	25.91	C
ATOM	5497	C	VAL	L	207	-18.592	53.451	79.304	1.00	25.77	C
ATOM	5498	O	VAL	L	207	-18.041	52.509	78.724	1.00	23.99	O
ATOM	5499	CB	VAL	L	207	-17.353	53.664	81.482	1.00	26.93	C
ATOM	5500	CG1	VAL	L	207	-16.640	54.867	80.002	1.00	28.46	C

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FIG. 53-86

ATOM	5502	N	THR	L	208	-19.104	54.488	78.663	1.00	26.57	N
ATOM	5503	CA	THR	L	208	-19.037	54.580	77.223	1.00	26.91	C
ATOM	5504	C	THR	L	208	-18.158	55.756	76.827	1.00	26.87	C
ATOM	5505	O	THR	L	208	-18.326	56.876	77.318	1.00	26.95	O
ATOM	5506	CB	THR	L	208	-20.457	54.749	76.599	1.00	27.63	C
ATOM	5507	OG1	THR	L	208	-21.355	53.779	77.163	1.00	27.17	O
ATOM	5508	CG2	THR	L	208	-20.399	54.543	75.089	1.00	25.39	C
ATOM	5509	N	LYS	L	209	-17.176	55.473	75.985	1.00	26.18	N
ATOM	5510	CA	LYS	L	209	-16.266	56.484	75.481	1.00	24.86	C
ATOM	5511	C	LYS	L	209	-16.485	56.409	73.989	1.00	25.02	C
ATOM	5512	O	LYS	L	209	-16.110	55.428	73.356	1.00	24.92	O
ATOM	5513	CB	LYS	L	209	-14.825	56.134	75.847	1.00	23.11	C
ATOM	5514	CG	LYS	L	209	-14.557	56.159	77.349	1.00	20.42	C
ATOM	5515	CD	LYS	L	209	-14.713	57.547	77.918	1.00	16.39	C
ATOM	5516	CE	LYS	L	209	-14.289	57.597	79.379	1.00	15.96	C
ATOM	5517	NZ	LYS	L	209	-14.204	58.997	79.884	1.00	13.55	N
ATOM	5518	N	SER	L	210	-17.164	57.417	73.451	1.00	26.26	N
ATOM	5519	CA	SER	L	210	-17.495	57.454	72.035	1.00	25.99	C
ATOM	5520	C	SER	L	210	-17.085	58.749	71.346	1.00	25.10	C
ATOM	5521	O	SER	L	210	-16.750	59.737	71.998	1.00	24.15	O
ATOM	5522	CB	SER	L	210	-19.006	57.245	71.885	1.00	26.74	C
ATOM	5523	OG	SER	L	210	-19.410	57.220	70.532	1.00	29.39	O
ATOM	5524	N	PHE	L	211	-17.118	58.723	70.018	1.00	25.06	N
ATOM	5525	CA	PHE	L	211	-16.792	59.884	69.202	1.00	24.49	C
ATOM	5526	C	PHE	L	211	-17.575	59.847	67.887	1.00	25.43	C
ATOM	5527	O	PHE	L	211	-18.606	59.171	67.794	1.00	24.52	O
ATOM	5528	CB	PHE	L	211	-15.281	60.005	68.967	1.00	22.18	C
ATOM	5529	CG	PHE	L	211	-14.722	58.992	68.019	1.00	19.69	C
ATOM	5530	CD1	PHE	L	211	-14.587	57.666	68.399	1.00	22.38	C
ATOM	5531	CD2	PHE	L	211	-14.299	59.375	66.754	1.00	19.66	C
ATOM	5532	CE1	PHE	L	211	-14.035	56.730	67.532	1.00	23.82	C
ATOM	5533	CE2	PHE	L	211	-13.748	58.458	65.880	1.00	21.68	C
ATOM	5534	CZ	PHE	L	211	-13.613	57.128	66.265	1.00	23.57	C
ATOM	5535	N	ASN	L	212	-17.088	60.543	66.864	1.00	27.12	N
ATOM	5536	CA	ASN	L	212	-17.804	60.589	65.599	1.00	29.02	C
ATOM	5537	C	ASN	L	212	-16.968	61.048	64.412	1.00	29.36	C
ATOM	5538	O	ASN	L	212	-15.887	61.620	64.577	1.00	30.52	O
ATOM	5539	CB	ASN	L	212	-19.020	61.506	65.739	1.00	30.60	C
ATOM	5540	CG	ASN	L	212	-18.664	62.839	66.362	1.00	33.09	C
ATOM	5541	OD1	ASN	L	212	-17.724	63.509	65.931	1.00	34.33	O
ATOM	5542	ND2	ASN	L	212	-19.391	63.218	67.398	1.00	34.80	N
ATOM	5543	N	ARG	L	213	-17.523	60.819	63.221	1.00	28.51	N
ATOM	5544	CA	ARG	L	213	-16.925	61.172	61.937	1.00	27.37	C
ATOM	5545	C	ARG	L	213	-15.935	60.112	61.479	1.00	27.24	C
ATOM	5546	O	ARG	L	213	-16.182	59.572	60.379	1.00	26.68	O
ATOM	5547	CB	ARG	L	213	-16.256	62.552	61.974	1.00	27.60	C
ATOM	5548	CG	ARG	L	213	-17.211	63.732	62.152	1.00	27.69	C
ATOM	5549	CD	ARG	L	213	-16.461	65.073	62.178	1.00	28.10	C
ATOM	5550	NE	ARG	L	213	-15.404	65.092	63.188	1.00	27.20	N
ATOM	5551	CZ	ARG	L	213	-14.103	65.179	62.917	1.00	26.87	C
ATOM	5552	NH1	ARG	L	213	-13.687	65.262	61.659	1.00	24.89	N
ATOM	5553	NH2	ARG	L	213	-13.217	65.159	63.906	1.00	27.14	N
TER	5554		ARG	L	213						
ATOM	5555	N	GLN	H	1	26.213	20.467	86.642	1.00	30.62	N
ATOM	5556	CA	GLN	H	1	25.208	21.506	86.279	1.00	30.11	C
ATOM	5557	C	GLN	H	1	25.492	21.995	84.875	1.00	28.53	C
ATOM	5558	O	GLN	H	1	26.450	22.733	84.656	1.00	28.92	O
ATOM	5559	CB	GLN	H	1	25.284	22.688	87.245	1.00	31.70	C
ATOM	5560	CG	GLN	H	1	24.677	22.432	88.599	1.00	34.69	C
ATOM	5561	CD	GLN	H	1	23.178	22.640	88.612	1.00	37.49	C
ATOM	5562	OE1	GLN	H	1	22.661	23.538	87.960	1.00	39.94	O
ATOM	5563	NE2	GLN	H	1	22.474	21.822	89.375	1.00	39.50	N
ATOM	5564	N	VAL	H	2	24.684	21.565	83.915	1.00	27.15	N
ATOM	5565	CA	VAL	H	2	24.884	21.992	82.538	1.00	25.30	C
ATOM	5566	C	VAL	H	2	24.331	23.394	82.259	1.00	24.46	C
ATOM	5567	O	VAL	H	2	23.586	23.958	83.071	1.00	24.66	O
ATOM	5568	CB	VAL	H	2	24.296	20.980	81.522	1.00	25.51	C
ATOM	5569	CG1	VAL	H	2	25.240	19.807	81.343	1.00	26.22	C
ATOM	5570	CG2	VAL	H	2	22.941	20.493	81.976	1.00	26.52	C
ATOM	5571	N	GLN	H	3	24.718	23.053	81.115	1.00	22.32	N

FIG. 53-87

ATOM	5573	C	GLN	H	3	23.779	25.101	79.264	1.00	17.85	C
ATOM	5574	O	GLN	H	3	24.567	24.928	78.334	1.00	18.21	O
ATOM	5575	CB	GLN	H	3	25.440	26.249	80.707	1.00	24.73	C
ATOM	5576	CG	GLN	H	3	25.999	26.486	82.097	1.00	31.68	C
ATOM	5577	CD	GLN	H	3	24.952	27.019	83.053	1.00	35.61	C
ATOM	5578	OE1	GLN	H	3	23.968	27.638	82.635	1.00	37.48	O
ATOM	5579	NE2	GLN	H	3	25.150	26.777	84.346	1.00	37.34	N
ATOM	5580	N	LEU	H	4	22.463	25.105	79.110	1.00	15.92	N
ATOM	5581	CA	LEU	H	4	21.837	24.915	77.806	1.00	13.88	C
ATOM	5582	C	LEU	H	4	21.557	26.214	77.063	1.00	12.34	C
ATOM	5583	O	LEU	H	4	20.797	27.057	77.543	1.00	12.85	O
ATOM	5584	CB	LEU	H	4	20.527	24.134	77.966	1.00	12.78	C
ATOM	5585	CG	LEU	H	4	20.551	22.875	78.841	1.00	10.51	C
ATOM	5586	CD1	LEU	H	4	19.148	22.302	78.905	1.00	8.09	C
ATOM	5587	CD2	LEU	H	4	21.549	21.852	78.295	1.00	10.28	C
ATOM	5588	N	LEU	H	5	22.163	26.354	75.887	1.00	10.72	N
ATOM	5589	CA	LEU	H	5	21.986	27.528	75.036	1.00	8.44	C
ATOM	5590	C	LEU	H	5	21.508	27.034	73.676	1.00	7.46	C
ATOM	5591	O	LEU	H	5	22.153	26.180	73.057	1.00	8.22	O
ATOM	5592	CB	LEU	H	5	23.298	28.324	74.910	1.00	8.68	C
ATOM	5593	CG	LEU	H	5	24.595	27.587	74.551	1.00	7.55	C
ATOM	5594	CD1	LEU	H	5	25.538	28.507	73.816	1.00	8.28	C
ATOM	5595	CD2	LEU	H	5	25.265	27.009	75.796	1.00	10.07	C
ATOM	5596	N	GLU	H	6	20.398	27.597	73.204	1.00	7.38	N
ATOM	5597	CA	GLU	H	6	19.775	27.192	71.938	1.00	6.70	C
ATOM	5598	C	GLU	H	6	19.929	28.157	70.771	1.00	7.54	C
ATOM	5599	O	GLU	H	6	20.386	29.287	70.941	1.00	8.78	O
ATOM	5600	CB	GLU	H	6	18.294	26.930	72.181	1.00	3.52	C
ATOM	5601	CG	GLU	H	6	18.038	26.284	73.528	1.00	3.07	C
ATOM	5602	CD	GLU	H	6	16.636	25.803	73.690	1.00	2.00	C
ATOM	5603	OE1	GLU	H	6	16.043	25.332	72.704	1.00	2.00	O
ATOM	5604	OE2	GLU	H	6	16.127	25.889	74.819	1.00	2.00	O
ATOM	5605	N	SER	H	7	19.510	27.706	69.592	1.00	7.96	N
ATOM	5606	CA	SER	H	7	19.582	28.492	68.364	1.00	8.44	C
ATOM	5607	C	SER	H	7	18.514	29.581	68.321	1.00	8.77	C
ATOM	5608	O	SER	H	7	17.502	29.486	69.008	1.00	9.13	O
ATOM	5609	CB	SER	H	7	19.467	27.569	67.143	1.00	11.38	C
ATOM	5610	OG	SER	H	7	18.512	26.535	67.352	1.00	15.43	O
ATOM	5611	N	GLY	H	8	18.739	30.601	67.495	1.00	7.57	N
ATOM	5612	CA	GLY	H	8	17.814	31.717	67.394	1.00	6.97	C
ATOM	5613	C	GLY	H	8	16.500	31.345	66.762	1.00	5.80	C
ATOM	5614	O	GLY	H	8	16.328	30.200	66.365	1.00	6.19	O
ATOM	5615	N	ALA	H	9	15.607	32.321	66.613	1.00	4.10	N
ATOM	5616	CA	ALA	H	9	14.288	32.082	66.037	1.00	5.03	C
ATOM	5617	C	ALA	H	9	14.295	31.591	64.581	1.00	5.79	C
ATOM	5618	O	ALA	H	9	15.226	31.874	63.821	1.00	7.48	O
ATOM	5619	CB	ALA	H	9	13.452	33.315	66.165	1.00	4.80	C
ATOM	5620	N	GLU	H	10	13.237	30.883	64.198	1.00	3.83	N
ATOM	5621	CA	GLU	H	10	13.104	30.333	62.851	1.00	3.26	C
ATOM	5622	C	GLU	H	10	11.787	30.743	62.232	1.00	3.25	C
ATOM	5623	O	GLU	H	10	10.751	30.728	62.887	1.00	5.55	O
ATOM	5624	CB	GLU	H	10	13.109	28.795	62.885	1.00	3.97	C
ATOM	5625	CG	GLU	H	10	14.443	28.128	63.180	1.00	2.24	C
ATOM	5626	CD	GLU	H	10	15.375	28.103	61.997	1.00	2.00	C
ATOM	5627	OE1	GLU	H	10	14.933	28.232	60.830	1.00	3.34	O
ATOM	5628	OE2	GLU	H	10	16.575	27.925	62.232	1.00	3.37	O
ATOM	5629	N	VAL	H	11	11.809	31.072	60.953	1.00	3.17	N
ATOM	5630	CA	VAL	H	11	10.591	31.433	60.252	1.00	5.01	C
ATOM	5631	C	VAL	H	11	10.587	30.415	59.122	1.00	4.61	C
ATOM	5632	O	VAL	H	11	11.561	30.328	58.373	1.00	3.89	O
ATOM	5633	CB	VAL	H	11	10.642	32.875	59.699	1.00	8.53	C
ATOM	5634	CG1	VAL	H	11	9.238	33.342	59.344	1.00	7.21	C
ATOM	5635	CG2	VAL	H	11	11.277	33.814	60.724	1.00	9.48	C
ATOM	5636	N	LYS	H	12	9.545	29.587	59.072	1.00	4.07	N
ATOM	5637	CA	LYS	H	12	9.420	28.538	58.072	1.00	5.19	C
ATOM	5638	C	LYS	H	12	8.045	28.563	57.420	1.00	5.91	C
ATOM	5639	O	LYS	H	12	7.065	28.902	58.077	1.00	8.34	O
ATOM	5640	CB	LYS	H	12	9.576	27.166	58.752	1.00	5.83	C
ATOM	5641	CG	LYS	H	12	10.920	26.885	59.393	1.00	2.00	C
ATOM	5642	CD	LYS	H	12	[illegible]	[illegible]	[illegible]	1.00	2.00	C

FIG. 53-88

ATOM	5644	NZ	LYS	H	12	14.489	26.810	58.321	1.00	6.51	N
ATOM	5645	N	LYS	H	13	7.956	28.202	56.142	1.00	5.24	N
ATOM	5646	CA	LYS	H	13	6.646	28.152	55.486	1.00	6.75	C
ATOM	5647	C	LYS	H	13	6.097	26.765	55.855	1.00	6.71	C
ATOM	5648	O	LYS	H	13	6.868	25.824	56.060	1.00	6.69	O
ATOM	5649	CB	LYS	H	13	6.762	28.264	53.955	1.00	7.21	C
ATOM	5650	CG	LYS	H	13	7.358	29.558	53.391	1.00	5.94	C
ATOM	5651	CD	LYS	H	13	6.434	30.739	53.593	1.00	9.27	C
ATOM	5652	CE	LYS	H	13	6.696	31.844	52.586	1.00	8.08	C
ATOM	5653	NZ	LYS	H	13	6.285	31.389	51.234	1.00	14.24	N
ATOM	5654	N	PRO	H	14	4.768	26.613	55.945	1.00	6.24	N
ATOM	5655	CA	PRO	H	14	4.247	25.288	56.301	1.00	5.61	C
ATOM	5656	C	PRO	H	14	4.558	24.213	55.263	1.00	5.99	C
ATOM	5657	O	PRO	H	14	4.224	24.341	54.089	1.00	6.85	O
ATOM	5658	CB	PRO	H	14	2.746	25.537	56.486	1.00	7.13	C
ATOM	5659	CG	PRO	H	14	2.475	26.763	55.637	1.00	7.66	C
ATOM	5660	CD	PRO	H	14	3.690	27.613	55.843	1.00	5.62	C
ATOM	5661	N	GLY	H	15	5.231	23.160	55.712	1.00	6.24	N
ATOM	5662	CA	GLY	H	15	5.608	22.066	54.836	1.00	3.56	C
ATOM	5663	C	GLY	H	15	7.106	21.841	54.889	1.00	3.60	C
ATOM	5664	O	GLY	H	15	7.603	20.830	54.392	1.00	4.72	O
ATOM	5665	N	SER	H	16	7.811	22.756	55.548	1.00	3.55	N
ATOM	5666	CA	SER	H	16	9.268	22.716	55.670	1.00	4.48	C
ATOM	5667	C	SER	H	16	9.789	21.893	56.857	1.00	6.62	C
ATOM	5668	O	SER	H	16	9.007	21.347	57.645	1.00	7.95	O
ATOM	5669	CB	SER	H	16	9.798	24.155	55.759	1.00	4.84	C
ATOM	5670	OG	SER	H	16	9.098	25.014	54.867	1.00	2.00	O
ATOM	5671	N	SER	H	17	11.112	21.778	56.952	1.00	8.11	N
ATOM	5672	CA	SER	H	17	11.766	21.033	58.026	1.00	9.36	C
ATOM	5673	C	SER	H	17	12.585	22.002	58.861	1.00	10.49	C
ATOM	5674	O	SER	H	17	13.310	22.845	58.324	1.00	13.72	O
ATOM	5675	CB	SER	H	17	12.731	19.984	57.463	1.00	8.58	C
ATOM	5676	OG	SER	H	17	12.092	19.077	56.583	1.00	11.68	O
ATOM	5677	N	VAL	H	18	12.514	21.853	60.173	1.00	9.20	N
ATOM	5678	CA	VAL	H	18	13.254	22.722	61.063	1.00	8.05	C
ATOM	5679	C	VAL	H	18	14.114	21.868	61.970	1.00	10.27	C
ATOM	5680	O	VAL	H	18	13.706	20.780	62.387	1.00	9.51	O
ATOM	5681	CB	VAL	H	18	12.311	23.587	61.923	1.00	7.91	C
ATOM	5682	CG1	VAL	H	18	11.629	22.743	63.029	1.00	3.28	C
ATOM	5683	CG2	VAL	H	18	13.076	24.759	62.496	1.00	8.24	C
ATOM	5684	N	LYS	H	19	15.323	22.346	62.235	1.00	12.29	N
ATOM	5685	CA	LYS	H	19	16.249	21.645	63.101	1.00	13.79	C
ATOM	5686	C	LYS	H	19	16.826	22.678	64.039	1.00	14.54	C
ATOM	5687	O	LYS	H	19	17.589	23.554	63.612	1.00	15.89	O
ATOM	5688	CB	LYS	H	19	17.373	20.970	62.299	1.00	14.50	C
ATOM	5689	CG	LYS	H	19	18.479	20.367	63.172	1.00	15.10	C
ATOM	5690	CD	LYS	H	19	19.433	19.495	62.392	1.00	13.35	C
ATOM	5691	CE	LYS	H	19	19.050	18.028	62.523	1.00	18.64	C
ATOM	5692	NZ	LYS	H	19	17.755	17.668	61.866	1.00	23.12	N
ATOM	5693	N	VAL	H	20	16.423	22.594	65.304	1.00	13.54	N
ATOM	5694	CA	VAL	H	20	16.892	23.518	66.334	1.00	11.88	C
ATOM	5695	C	VAL	H	20	17.949	22.804	67.177	1.00	9.59	C
ATOM	5696	O	VAL	H	20	17.826	21.609	67.399	1.00	10.23	O
ATOM	5697	CB	VAL	H	20	15.703	23.993	67.191	1.00	12.27	C
ATOM	5698	CG1	VAL	H	20	14.670	24.674	66.298	1.00	9.57	C
ATOM	5699	CG2	VAL	H	20	15.054	22.818	67.887	1.00	13.94	C
ATOM	5700	N	SER	H	21	19.004	23.510	67.581	1.00	7.81	N
ATOM	5701	CA	SER	H	21	20.091	22.917	68.370	1.00	6.84	C
ATOM	5702	C	SER	H	21	20.080	23.367	69.816	1.00	6.68	C
ATOM	5703	O	SER	H	21	19.492	24.392	70.147	1.00	8.90	O
ATOM	5704	CB	SER	H	21	21.465	23.253	67.765	1.00	7.77	C
ATOM	5705	OG	SER	H	21	21.991	24.507	68.211	1.00	6.16	O
ATOM	5706	N	CYS	H	22	20.836	22.670	70.653	1.00	6.28	N
ATOM	5707	CA	CYS	H	22	20.903	22.996	72.069	1.00	7.75	C
ATOM	5708	C	CYS	H	22	22.274	22.607	72.618	1.00	7.86	C
ATOM	5709	O	CYS	H	22	22.495	21.456	73.001	1.00	8.34	O
ATOM	5710	CB	CYS	H	22	19.800	22.244	72.803	1.00	10.65	C
ATOM	5711	SG	CYS	H	22	19.857	22.267	74.625	1.00	16.65	S
ATOM	5712	N	LYS	H	23	23.193	23.571	72.627	1.00	8.06	N
ATOM	5713	CA	LYS	H	23	24.559	23.359	73.101	1.00	8.11	C

FIG. 53-89

ATOM	5715	O	LYS	H	23	24.416	24.136	75.376	1.00	10.29	O
ATOM	5716	CB	LYS	H	23	25.436	24.538	72.675	1.00	6.14	C
ATOM	5717	CG	LYS	H	23	26.885	24.185	72.370	1.00	6.72	C
ATOM	5718	CD	LYS	H	23	26.982	23.294	71.141	1.00	9.64	C
ATOM	5719	CE	LYS	H	23	26.287	23.912	69.927	1.00	11.78	C
ATOM	5720	NZ	LYS	H	23	26.297	23.010	68.743	1.00	10.31	N
ATOM	5721	N	ALA	H	24	24.925	21.955	75.054	1.00	8.98	N
ATOM	5722	CA	ALA	H	24	25.049	21.619	76.476	1.00	9.53	C
ATOM	5723	C	ALA	H	24	26.497	21.789	76.937	1.00	10.70	C
ATOM	5724	O	ALA	H	24	27.420	21.260	76.330	1.00	11.55	O
ATOM	5725	CB	ALA	H	24	24.595	20.195	76.720	1.00	7.15	C
ATOM	5726	N	SER	H	25	26.698	22.515	78.023	1.00	12.78	N
ATOM	5727	CA	SER	H	25	28.044	22.742	78.518	1.00	14.78	C
ATOM	5728	C	SER	H	25	28.071	22.741	80.033	1.00	14.58	C
ATOM	5729	O	SER	H	25	27.024	22.852	80.662	1.00	13.09	O
ATOM	5730	CB	SER	H	25	28.574	24.069	77.972	1.00	17.62	C
ATOM	5731	OG	SER	H	25	27.614	25.105	78.103	1.00	22.32	O
ATOM	5732	N	GLY	H	26	29.255	22.541	80.608	1.00	15.92	N
ATOM	5733	CA	GLY	H	26	29.396	22.548	82.056	1.00	17.21	C
ATOM	5734	C	GLY	H	26	29.420	21.220	82.795	1.00	18.55	C
ATOM	5735	O	GLY	H	26	29.938	21.141	83.910	1.00	19.33	O
ATOM	5736	N	ASP	H	27	28.901	20.164	82.182	1.00	19.59	N
ATOM	5737	CA	ASP	H	27	28.867	18.862	82.841	1.00	20.42	C
ATOM	5738	C	ASP	H	27	28.865	17.725	81.824	1.00	19.89	C
ATOM	5739	O	ASP	H	27	28.167	17.816	80.806	1.00	20.24	O
ATOM	5740	CB	ASP	H	27	27.592	18.764	83.690	1.00	21.74	C
ATOM	5741	CG	ASP	H	27	27.873	18.502	85.152	1.00	22.03	C
ATOM	5742	OD1	ASP	H	27	28.419	19.391	85.833	1.00	25.42	O
ATOM	5743	OD2	ASP	H	27	27.509	17.421	85.648	1.00	24.27	O
ATOM	5744	N	THR	H	28	29.630	16.665	82.109	1.00	18.47	N
ATOM	5745	CA	THR	H	28	29.729	15.460	81.265	1.00	15.68	C
ATOM	5746	C	THR	H	28	28.413	15.173	80.540	1.00	15.10	C
ATOM	5747	O	THR	H	28	27.528	14.503	81.074	1.00	16.73	O
ATOM	5748	CB	THR	H	28	30.057	14.197	82.110	1.00	14.61	C
ATOM	5749	OG1	THR	H	28	31.190	14.438	82.948	1.00	16.36	O
ATOM	5750	CG2	THR	H	28	30.371	13.026	81.212	1.00	13.15	C
ATOM	5751	N	PHE	H	29	28.332	15.643	79.303	1.00	13.46	N
ATOM	5752	CA	PHE	H	29	27.159	15.511	78.437	1.00	13.09	C
ATOM	5753	C	PHE	H	29	26.405	14.179	78.469	1.00	13.89	C
ATOM	5754	O	PHE	H	29	25.177	14.171	78.561	1.00	13.56	O
ATOM	5755	CB	PHE	H	29	27.585	15.838	76.998	1.00	13.57	C
ATOM	5756	CG	PHE	H	29	26.467	15.823	75.991	1.00	10.76	C
ATOM	5757	CD1	PHE	H	29	25.376	16.670	76.125	1.00	12.04	C
ATOM	5758	CD2	PHE	H	29	26.555	15.028	74.858	1.00	11.09	C
ATOM	5759	CE1	PHE	H	29	24.396	16.734	75.140	1.00	10.05	C
ATOM	5760	CE2	PHE	H	29	25.579	15.083	73.867	1.00	10.65	C
ATOM	5761	CZ	PHE	H	29	24.498	15.943	74.010	1.00	11.71	C
ATOM	5762	N	ILE	H	30	27.143	13.070	78.394	1.00	14.74	N
ATOM	5763	CA	ILE	H	30	26.554	11.724	78.367	1.00	14.10	C
ATOM	5764	C	ILE	H	30	25.740	11.336	79.583	1.00	13.21	C
ATOM	5765	O	ILE	H	30	24.757	10.593	79.460	1.00	12.68	O
ATOM	5766	CB	ILE	H	30	27.614	10.606	78.183	1.00	15.32	C
ATOM	5767	CG1	ILE	H	30	29.008	11.088	78.599	1.00	17.77	C
ATOM	5768	CG2	ILE	H	30	27.552	10.049	76.781	1.00	15.71	C
ATOM	5769	CD1	ILE	H	30	30.129	10.067	78.345	1.00	19.27	C
ATOM	5770	N	ARG	H	31	26.148	11.847	80.746	1.00	10.64	N
ATOM	5771	CA	ARG	H	31	25.494	11.545	82.022	1.00	6.72	C
ATOM	5772	C	ARG	H	31	24.125	12.200	82.201	1.00	4.71	C
ATOM	5773	O	ARG	H	31	23.568	12.151	83.288	1.00	4.96	O
ATOM	5774	CB	ARG	H	31	26.398	11.978	83.181	1.00	6.64	C
ATOM	5775	CG	ARG	H	31	27.847	11.483	83.120	1.00	7.34	C
ATOM	5776	CD	ARG	H	31	28.625	11.984	84.345	1.00	11.53	C
ATOM	5777	NE	ARG	H	31	30.059	11.651	84.342	1.00	12.07	N
ATOM	5778	CZ	ARG	H	31	30.604	10.661	85.054	1.00	12.53	C
ATOM	5779	NH1	ARG	H	31	29.837	9.899	85.819	1.00	10.53	N
ATOM	5780	NH2	ARG	H	31	31.919	10.447	85.028	1.00	11.18	N
ATOM	5781	N	TYR	H	32	23.589	12.794	81.138	1.00	3.90	N
ATOM	5782	CA	TYR	H	32	22.309	13.493	81.157	1.00	2.81	C
ATOM	5783	C	TYR	H	32	21.437	12.987	80.023	1.00	3.71	C
ATOM	5784	O	TYR	H	32	21.961	12.487	79.017	1.00	3.40	O

FIG. 53-90

ATOM	5786	CG	TYR	H	32	23.120	15.821	82.001	1.00	7.39	C
ATOM	5787	CD1	TYR	H	32	24.490	15.803	82.281	1.00	6.34	C
ATOM	5788	CD2	TYR	H	32	22.299	16.630	82.781	1.00	6.97	C
ATOM	5789	CE1	TYR	H	32	25.017	16.571	83.318	1.00	10.53	C
ATOM	5790	CE2	TYR	H	32	22.802	17.395	83.806	1.00	10.74	C
ATOM	5791	CZ	TYR	H	32	24.158	17.373	84.086	1.00	13.42	C
ATOM	5792	OH	TYR	H	32	24.619	18.143	85.144	1.00	15.09	O
ATOM	5793	N	SER	H	33	20.117	13.129	80.173	1.00	3.85	N
ATOM	5794	CA	SER	H	33	19.182	12.755	79.113	1.00	5.31	C
ATOM	5795	C	SER	H	33	18.376	14.012	78.804	1.00	6.65	C
ATOM	5796	O	SER	H	33	17.848	14.648	79.718	1.00	6.29	O
ATOM	5797	CB	SER	H	33	18.280	11.591	79.521	1.00	5.99	C
ATOM	5798	OG	SER	H	33	17.341	11.937	80.508	1.00	3.85	O
ATOM	5799	N	PHE	H	34	18.315	14.391	77.530	1.00	7.73	N
ATOM	5800	CA	PHE	H	34	17.611	15.610	77.126	1.00	7.57	C
ATOM	5801	C	PHE	H	34	16.258	15.426	76.464	1.00	7.43	C
ATOM	5802	O	PHE	H	34	16.065	14.551	75.626	1.00	8.72	O
ATOM	5803	CB	PHE	H	34	18.518	16.478	76.268	1.00	7.39	C
ATOM	5804	CG	PHE	H	34	19.806	16.826	76.941	1.00	7.62	C
ATOM	5805	CD1	PHE	H	34	19.878	17.891	77.820	1.00	8.01	C
ATOM	5806	CD2	PHE	H	34	20.939	16.053	76.730	1.00	8.52	C
ATOM	5807	CE1	PHE	H	34	21.057	18.194	78.477	1.00	8.53	C
ATOM	5808	CE2	PHE	H	34	22.122	16.345	77.382	1.00	8.34	C
ATOM	5809	CZ	PHE	H	34	22.179	17.413	78.259	1.00	9.73	C
ATOM	5810	N	THR	H	35	15.345	16.316	76.827	1.00	8.01	N
ATOM	5811	CA	THR	H	35	13.976	16.310	76.361	1.00	8.74	C
ATOM	5812	C	THR	H	35	13.682	17.643	75.691	1.00	10.09	C
ATOM	5813	O	THR	H	35	14.391	18.635	75.906	1.00	11.27	O
ATOM	5814	CB	THR	H	35	13.018	16.195	77.571	1.00	9.79	C
ATOM	5815	OG1	THR	H	35	13.450	15.141	78.441	1.00	9.92	O
ATOM	5816	CG2	THR	H	35	11.596	15.916	77.116	1.00	9.69	C
ATOM	5817	N	TRP	H	36	12.627	17.664	74.885	1.00	9.20	N
ATOM	5818	CA	TRP	H	36	12.198	18.874	74.210	1.00	7.34	C
ATOM	5819	C	TRP	H	36	10.757	19.148	74.605	1.00	7.87	C
ATOM	5820	O	TRP	H	36	9.906	18.247	74.563	1.00	8.30	O
ATOM	5821	CB	TRP	H	36	12.318	18.732	72.700	1.00	4.76	C
ATOM	5822	CG	TRP	H	36	13.720	18.892	72.206	1.00	3.17	C
ATOM	5823	CD1	TRP	H	36	14.635	17.904	71.996	1.00	2.08	C
ATOM	5824	CD2	TRP	H	36	14.366	20.119	71.848	1.00	3.73	C
ATOM	5825	NE1	TRP	H	36	15.808	18.433	71.525	1.00	2.00	N
ATOM	5826	CE2	TRP	H	36	15.674	19.793	71.422	1.00	4.34	C
ATOM	5827	CE3	TRP	H	36	13.965	21.464	71.836	1.00	2.18	C
ATOM	5828	CZ2	TRP	H	36	16.595	20.769	70.994	1.00	3.76	C
ATOM	5829	CZ3	TRP	H	36	14.881	22.436	71.409	1.00	3.07	C
ATOM	5830	CH2	TRP	H	36	16.178	22.079	70.990	1.00	2.86	C
ATOM	5831	N	VAL	H	37	10.513	20.376	75.059	1.00	7.63	N
ATOM	5832	CA	VAL	H	37	9.193	20.824	75.474	1.00	6.92	C
ATOM	5833	C	VAL	H	37	8.840	22.050	74.630	1.00	7.51	C
ATOM	5834	O	VAL	H	37	9.632	22.988	74.522	1.00	6.76	O
ATOM	5835	CB	VAL	H	37	9.174	21.206	76.978	1.00	6.04	C
ATOM	5836	CG1	VAL	H	37	7.813	21.754	77.371	1.00	5.15	C
ATOM	5837	CG2	VAL	H	37	9.507	19.999	77.834	1.00	5.87	C
ATOM	5838	N	ARG	H	38	7.677	22.010	73.989	1.00	8.71	N
ATOM	5839	CA	ARG	H	38	7.211	23.119	73.148	1.00	7.89	C
ATOM	5840	C	ARG	H	38	6.103	23.862	73.865	1.00	8.66	C
ATOM	5841	O	ARG	H	38	5.390	23.288	74.703	1.00	8.92	O
ATOM	5842	CB	ARG	H	38	6.678	22.613	71.795	1.00	5.20	C
ATOM	5843	CG	ARG	H	38	5.619	21.528	71.910	1.00	4.10	C
ATOM	5844	CD	ARG	H	38	4.557	21.585	70.810	1.00	2.00	C
ATOM	5845	NE	ARG	H	38	5.067	21.324	69.467	1.00	5.03	N
ATOM	5846	CZ	ARG	H	38	4.311	20.873	68.466	1.00	5.96	C
ATOM	5847	NH1	ARG	H	38	3.020	20.616	68.660	1.00	5.70	N
ATOM	5848	NH2	ARG	H	38	4.823	20.763	67.250	1.00	2.54	N
ATOM	5849	N	GLN	H	39	5.947	25.136	73.531	1.00	9.12	N
ATOM	5850	CA	GLN	H	39	4.904	25.946	74.149	1.00	9.49	C
ATOM	5851	C	GLN	H	39	4.377	26.934	73.125	1.00	10.88	C
ATOM	5852	O	GLN	H	39	5.129	27.747	72.588	1.00	11.68	O
ATOM	5853	CB	GLN	H	39	5.451	26.680	75.365	1.00	7.51	C
ATOM	5854	CG	GLN	H	39	4.394	27.331	76.241	1.00	6.05	C
ATOM	5855	CD	GLN	H	39	5.015	28.003	77.383	1.00	2.75	C

FIG. 53-91

ATOM	5857	NE2	GLN	H	39	4.335	28.135	78.517	1.00	4.69	N
ATOM	5858	N	ALA	H	40	3.102	26.783	72.789	1.00	11.12	N
ATOM	5859	CA	ALA	H	40	2.451	27.648	71.832	1.00	11.60	C
ATOM	5860	C	ALA	H	40	2.036	28.922	72.551	1.00	12.54	C
ATOM	5861	O	ALA	H	40	1.617	28.878	73.711	1.00	11.95	O
ATOM	5862	CB	ALA	H	40	1.227	26.946	71.257	1.00	12.94	C
ATOM	5863	N	PRO	H	41	2.122	30.073	71.863	1.00	13.85	N
ATOM	5864	CA	PRO	H	41	1.776	31.406	72.355	1.00	14.71	C
ATOM	5865	C	PRO	H	41	0.992	31.547	73.659	1.00	16.10	C
ATOM	5866	O	PRO	H	41	1.566	31.942	74.684	1.00	16.71	O
ATOM	5867	CB	PRO	H	41	1.047	31.993	71.165	1.00	14.20	C
ATOM	5868	CG	PRO	H	41	1.977	31.579	70.052	1.00	15.51	C
ATOM	5869	CD	PRO	H	41	2.453	30.154	70.429	1.00	13.73	C
ATOM	5870	N	GLY	H	42	-0.303	31.241	73.634	1.00	16.21	N
ATOM	5871	CA	GLY	H	42	-1.095	31.387	74.845	1.00	17.00	C
ATOM	5872	C	GLY	H	42	-1.464	30.098	75.545	1.00	16.65	C
ATOM	5873	O	GLY	H	42	-2.388	30.074	76.376	1.00	15.76	O
ATOM	5874	N	GLN	H	43	-0.738	29.031	75.223	1.00	15.80	N
ATOM	5875	CA	GLN	H	43	-1.003	27.719	75.811	1.00	15.55	C
ATOM	5876	C	GLN	H	43	0.085	27.280	76.791	1.00	13.04	C
ATOM	5877	O	GLN	H	43	0.962	28.067	77.167	1.00	13.60	O
ATOM	5878	CB	GLN	H	43	-1.159	26.669	74.708	1.00	17.67	C
ATOM	5879	CG	GLN	H	43	-2.090	27.079	73.597	1.00	23.37	C
ATOM	5880	CD	GLN	H	43	-3.421	27.567	74.120	1.00	29.07	C
ATOM	5881	OE1	GLN	H	43	-3.669	28.773	74.190	1.00	32.20	O
ATOM	5882	NE2	GLN	H	43	-4.291	26.634	74.490	1.00	32.38	N
ATOM	5883	N	GLY	H	44	0.013	26.020	77.204	1.00	9.85	N
ATOM	5884	CA	GLY	H	44	0.979	25.486	78.136	1.00	7.51	C
ATOM	5885	C	GLY	H	44	2.035	24.598	77.514	1.00	6.25	C
ATOM	5886	O	GLY	H	44	2.139	24.495	76.284	1.00	4.79	O
ATOM	5887	N	LEU	H	45	2.809	23.952	78.387	1.00	5.54	N
ATOM	5888	CA	LEU	H	45	3.897	23.050	78.011	1.00	4.49	C
ATOM	5889	C	LEU	H	45	3.410	21.717	77.419	1.00	4.02	C
ATOM	5890	O	LEU	H	45	2.361	21.209	77.813	1.00	3.67	O
ATOM	5891	CB	LEU	H	45	4.752	22.761	79.243	1.00	4.27	C
ATOM	5892	CG	LEU	H	45	5.391	23.917	80.015	1.00	2.21	C
ATOM	5893	CD1	LEU	H	45	5.956	23.392	81.334	1.00	2.00	C
ATOM	5894	CD2	LEU	H	45	6.477	24.576	79.193	1.00	2.87	C
ATOM	5895	N	GLU	H	46	4.177	21.175	76.476	1.00	3.36	N
ATOM	5896	CA	GLU	H	46	3.873	19.902	75.813	1.00	4.62	C
ATOM	5897	C	GLU	H	46	5.141	19.074	75.579	1.00	4.79	C
ATOM	5898	O	GLU	H	46	6.088	19.519	74.917	1.00	5.47	O
ATOM	5899	CB	GLU	H	46	3.179	20.128	74.461	1.00	5.98	C
ATOM	5900	CG	GLU	H	46	3.287	18.939	73.500	1.00	2.77	C
ATOM	5901	CD	GLU	H	46	2.415	19.066	72.264	1.00	2.40	C
ATOM	5902	OE1	GLU	H	46	1.191	19.249	72.407	1.00	2.00	O
ATOM	5903	OE2	GLU	H	46	2.945	18.947	71.139	1.00	3.18	O
ATOM	5904	N	TRP	H	47	5.140	17.860	76.110	1.00	4.47	N
ATOM	5905	CA	TRP	H	47	6.264	16.947	75.972	1.00	4.38	C
ATOM	5906	C	TRP	H	47	6.284	16.461	74.521	1.00	4.97	C
ATOM	5907	O	TRP	H	47	5.256	16.006	74.005	1.00	5.28	O
ATOM	5908	CB	TRP	H	47	6.054	15.767	76.933	1.00	6.19	C
ATOM	5909	CG	TRP	H	47	7.283	14.946	77.262	1.00	7.45	C
ATOM	5910	CD1	TRP	H	47	8.253	15.249	78.182	1.00	6.44	C
ATOM	5911	CD2	TRP	H	47	7.672	13.694	76.664	1.00	4.88	C
ATOM	5912	NE1	TRP	H	47	9.220	14.263	78.186	1.00	6.10	N
ATOM	5913	CE2	TRP	H	47	8.890	13.302	77.266	1.00	2.74	C
ATOM	5914	CE3	TRP	H	47	7.117	12.871	75.677	1.00	5.15	C
ATOM	5915	CZ2	TRP	H	47	9.559	12.131	76.907	1.00	2.54	C
ATOM	5916	CZ3	TRP	H	47	7.787	11.700	75.320	1.00	3.52	C
ATOM	5917	CH2	TRP	H	47	8.994	11.345	75.934	1.00	3.72	C
ATOM	5918	N	MET	H	48	7.426	16.590	73.853	1.00	4.75	N
ATOM	5919	CA	MET	H	48	7.552	16.134	72.467	1.00	4.88	C
ATOM	5920	C	MET	H	48	8.335	14.829	72.376	1.00	7.28	C
ATOM	5921	O	MET	H	48	8.014	13.960	71.557	1.00	6.58	O
ATOM	5922	CB	MET	H	48	8.279	17.163	71.617	1.00	4.03	C
ATOM	5923	CG	MET	H	48	7.689	18.546	71.642	1.00	4.05	C
ATOM	5924	SD	MET	H	48	8.593	19.532	70.478	1.00	2.86	S
ATOM	5925	CE	MET	H	48	7.829	18.949	68.955	1.00	2.92	C
ATOM	5926	N	GLY	H	49	9.396	14.724	73.175	1.00	8.91	N

FIG. 53-92

ATOM	5928	C	GLY	H	49	11.461	13.660	74.027	1.00	10.48	C
ATOM	5929	O	GLY	H	49	11.801	14.760	74.467	1.00	12.06	O
ATOM	5930	N	ARG	H	50	12.161	12.549	74.235	1.00	10.06	N
ATOM	5931	CA	ARG	H	50	13.365	12.547	75.058	1.00	9.26	C
ATOM	5932	C	ARG	H	50	14.386	11.544	74.569	1.00	9.54	C
ATOM	5933	O	ARG	H	50	14.031	10.419	74.229	1.00	12.18	O
ATOM	5934	CB	ARG	H	50	12.989	12.198	76.491	1.00	9.69	C
ATOM	5935	CG	ARG	H	50	14.156	11.905	77.402	1.00	9.78	C
ATOM	5936	CD	ARG	H	50	13.658	11.718	78.807	1.00	10.17	C
ATOM	5937	NE	ARG	H	50	14.697	11.207	79.689	1.00	13.80	N
ATOM	5938	CZ	ARG	H	50	14.762	9.950	80.118	1.00	13.53	C
ATOM	5939	NH1	ARG	H	50	13.849	9.067	79.729	1.00	12.57	N
ATOM	5940	NH2	ARG	H	50	15.696	9.596	80.995	1.00	14.85	N
ATOM	5941	N	ILE	H	51	15.655	11.932	74.564	1.00	8.81	N
ATOM	5942	CA	ILE	H	51	16.714	11.033	74.142	1.00	7.44	C
ATOM	5943	C	ILE	H	51	17.628	10.665	75.316	1.00	9.24	C
ATOM	5944	O	ILE	H	51	17.962	11.501	76.163	1.00	10.60	O
ATOM	5945	CB	ILE	H	51	17.536	11.601	72.941	1.00	5.75	C
ATOM	5946	CG1	ILE	H	51	18.647	10.621	72.547	1.00	3.54	C
ATOM	5947	CG2	ILE	H	51	18.060	12.995	73.243	1.00	4.92	C
ATOM	5948	CD1	ILE	H	51	19.577	11.116	71.468	1.00	2.00	C
ATOM	5949	N	ILE	H	52	17.942	9.375	75.399	1.00	9.98	N
ATOM	5950	CA	ILE	H	52	18.819	8.807	76.420	1.00	7.84	C
ATOM	5951	C	ILE	H	52	20.234	8.905	75.833	1.00	7.68	C
ATOM	5952	O	ILE	H	52	20.756	7.962	75.230	1.00	5.79	O
ATOM	5953	CB	ILE	H	52	18.410	7.324	76.701	1.00	6.65	C
ATOM	5954	CG1	ILE	H	52	16.951	7.267	77.174	1.00	4.76	C
ATOM	5955	CG2	ILE	H	52	19.343	6.679	77.718	1.00	4.82	C
ATOM	5956	CD1	ILE	H	52	16.406	5.865	77.394	1.00	3.25	C
ATOM	5957	N	THR	H	53	20.829	10.076	75.996	1.00	9.03	N
ATOM	5958	CA	THR	H	53	22.159	10.394	75.471	1.00	10.89	C
ATOM	5959	C	THR	H	53	23.320	9.376	75.572	1.00	12.64	C
ATOM	5960	O	THR	H	53	24.366	9.571	74.940	1.00	14.11	O
ATOM	5961	CB	THR	H	53	22.634	11.743	76.045	1.00	9.91	C
ATOM	5962	OG1	THR	H	53	21.492	12.583	76.290	1.00	9.80	O
ATOM	5963	CG2	THR	H	53	23.574	12.437	75.059	1.00	5.63	C
ATOM	5964	N	ILE	H	54	23.173	8.325	76.374	1.00	12.61	N
ATOM	5965	CA	ILE	H	54	24.239	7.326	76.507	1.00	12.19	C
ATOM	5966	C	ILE	H	54	24.081	6.241	75.429	1.00	12.10	C
ATOM	5967	O	ILE	H	54	25.050	5.831	74.795	1.00	10.19	O
ATOM	5968	CB	ILE	H	54	24.274	6.718	77.961	1.00	11.70	C
ATOM	5969	CG1	ILE	H	54	25.359	5.642	78.094	1.00	13.60	C
ATOM	5970	CG2	ILE	H	54	22.920	6.152	78.353	1.00	11.80	C
ATOM	5971	CD1	ILE	H	54	26.785	6.172	78.083	1.00	12.85	C
ATOM	5972	N	LEU	H	55	22.830	5.866	75.179	1.00	13.29	N
ATOM	5973	CA	LEU	H	55	22.435	4.847	74.200	1.00	12.91	C
ATOM	5974	C	LEU	H	55	22.031	5.402	72.831	1.00	14.22	C
ATOM	5975	O	LEU	H	55	22.029	4.664	71.843	1.00	16.37	O
ATOM	5976	CB	LEU	H	55	21.226	4.065	74.727	1.00	10.80	C
ATOM	5977	CG	LEU	H	55	21.307	2.919	75.729	1.00	9.21	C
ATOM	5978	CD1	LEU	H	55	22.658	2.893	76.415	1.00	10.96	C
ATOM	5979	CD2	LEU	H	55	20.158	3.047	76.719	1.00	5.46	C
ATOM	5980	N	ASP	H	56	21.617	6.665	72.793	1.00	15.31	N
ATOM	5981	CA	ASP	H	56	21.163	7.314	71.564	1.00	16.12	C
ATOM	5982	C	ASP	H	56	19.779	6.798	71.182	1.00	15.94	C
ATOM	5983	O	ASP	H	56	19.468	6.640	69.999	1.00	15.80	O
ATOM	5984	CB	ASP	H	56	22.132	7.088	70.405	1.00	18.24	C
ATOM	5985	CG	ASP	H	56	23.430	7.818	70.586	1.00	22.61	C
ATOM	5986	OD1	ASP	H	56	23.401	9.058	70.769	1.00	26.74	O
ATOM	5987	OD2	ASP	H	56	24.484	7.151	70.546	1.00	24.77	O
ATOM	5988	N	VAL	H	57	18.959	6.507	72.187	1.00	14.68	N
ATOM	5989	CA	VAL	H	57	17.610	6.012	71.936	1.00	13.55	C
ATOM	5990	C	VAL	H	57	16.605	7.019	72.450	1.00	12.46	C
ATOM	5991	O	VAL	H	57	16.552	7.297	73.647	1.00	11.82	O
ATOM	5992	CB	VAL	H	57	17.347	4.607	72.583	1.00	13.25	C
ATOM	5993	CG1	VAL	H	57	18.117	3.531	71.845	1.00	12.13	C
ATOM	5994	CG2	VAL	H	57	17.759	4.600	74.036	1.00	14.04	C
ATOM	5995	N	ALA	H	58	15.861	7.616	71.525	1.00	11.71	N
ATOM	5996	CA	ALA	H	58	14.847	8.603	71.873	1.00	10.71	C
ATOM	5997	C	ALA	H	58	13.466	7.968	71.821	1.00	10.16	C

FIG. 53-93

ATOM	5999	CB	ALA	H	58	14.918	9.792	70.922	1.00	11.97	C
ATOM	6000	N	HIS	H	59	12.554	8.475	72.640	1.00	8.76	N
ATOM	6001	CA	HIS	H	59	11.190	7.973	72.720	1.00	9.14	C
ATOM	6002	C	HIS	H	59	10.303	9.201	72.578	1.00	12.02	C
ATOM	6003	O	HIS	H	59	10.303	10.074	73.455	1.00	14.15	O
ATOM	6004	CB	HIS	H	59	10.977	7.298	74.071	1.00	8.02	C
ATOM	6005	CG	HIS	H	59	11.842	6.099	74.276	1.00	7.40	C
ATOM	6006	ND1	HIS	H	59	13.199	6.142	74.480	1.00	8.73	N
ATOM	6007	CD2	HIS	H	59	11.522	4.776	74.260	1.00	7.19	C
ATOM	6008	CE1	HIS	H	59	13.658	4.888	74.578	1.00	5.53	C
ATOM	6009	NE2	HIS	H	59	12.674	4.022	74.449	1.00	5.46	N
ATOM	6010	N	TYR	H	60	9.577	9.282	71.464	1.00	11.83	N
ATOM	6011	CA	TYR	H	60	8.731	10.435	71.167	1.00	11.67	C
ATOM	6012	C	TYR	H	60	7.289	10.281	71.577	1.00	11.43	C
ATOM	6013	O	TYR	H	60	6.823	9.175	71.797	1.00	13.83	O
ATOM	6014	CB	TYR	H	60	8.798	10.756	69.680	1.00	13.50	C
ATOM	6015	CG	TYR	H	60	10.207	10.763	69.133	1.00	14.95	C
ATOM	6016	CD1	TYR	H	60	11.093	11.784	69.458	1.00	14.67	C
ATOM	6017	CD2	TYR	H	60	10.664	9.728	68.310	1.00	13.95	C
ATOM	6018	CE1	TYR	H	60	12.391	11.773	68.981	1.00	14.47	C
ATOM	6019	CE2	TYR	H	60	11.965	9.715	67.832	1.00	12.16	C
ATOM	6020	CZ	TYR	H	60	12.819	10.738	68.172	1.00	12.33	C
ATOM	6021	OH	TYR	H	60	14.107	10.739	67.704	1.00	13.46	O
ATOM	6022	N	ALA	H	61	6.583	11.403	71.633	1.00	11.41	N
ATOM	6023	CA	ALA	H	61	5.181	11.434	72.026	1.00	13.02	C
ATOM	6024	C	ALA	H	61	4.270	10.905	70.911	1.00	14.85	C
ATOM	6025	O	ALA	H	61	4.409	11.277	69.745	1.00	16.00	O
ATOM	6026	CB	ALA	H	61	4.782	12.857	72.404	1.00	11.91	C
ATOM	6027	N	PRO	H	62	3.305	10.046	71.261	1.00	15.17	N
ATOM	6028	CA	PRO	H	62	2.386	9.485	70.271	1.00	15.38	C
ATOM	6029	C	PRO	H	62	1.406	10.499	69.650	1.00	17.18	C
ATOM	6030	O	PRO	H	62	0.206	10.502	69.956	1.00	19.60	O
ATOM	6031	CB	PRO	H	62	1.683	8.386	71.061	1.00	14.73	C
ATOM	6032	CG	PRO	H	62	1.692	8.924	72.459	1.00	16.02	C
ATOM	6033	CD	PRO	H	62	3.078	9.451	72.589	1.00	15.20	C
ATOM	6034	N	HIS	H	63	1.943	11.359	68.788	1.00	16.39	N
ATOM	6035	CA	HIS	H	63	1.195	12.387	68.060	1.00	15.11	C
ATOM	6036	C	HIS	H	63	2.208	13.130	67.189	1.00	14.22	C
ATOM	6037	O	HIS	H	63	1.865	13.741	66.181	1.00	13.83	O
ATOM	6038	CB	HIS	H	63	0.416	13.338	69.002	1.00	14.89	C
ATOM	6039	CG	HIS	H	63	1.216	14.480	69.565	1.00	15.15	C
ATOM	6040	ND1	HIS	H	63	1.762	14.455	70.831	1.00	15.98	N
ATOM	6041	CD2	HIS	H	63	1.480	15.713	69.071	1.00	13.13	C
ATOM	6042	CE1	HIS	H	63	2.327	15.621	71.095	1.00	12.59	C
ATOM	6043	NE2	HIS	H	63	2.169	16.401	70.043	1.00	13.03	N
ATOM	6044	N	LEU	H	64	3.465	13.067	67.611	1.00	13.05	N
ATOM	6045	CA	LEU	H	64	4.582	13.684	66.913	1.00	12.91	C
ATOM	6046	C	LEU	H	64	5.381	12.577	66.233	1.00	14.95	C
ATOM	6047	O	LEU	H	64	6.140	12.827	65.294	1.00	16.52	O
ATOM	6048	CB	LEU	H	64	5.474	14.400	67.926	1.00	12.13	C
ATOM	6049	CG	LEU	H	64	5.459	15.928	67.970	1.00	9.82	C
ATOM	6050	CD1	LEU	H	64	4.109	16.479	67.568	1.00	10.49	C
ATOM	6051	CD2	LEU	H	64	5.821	16.377	69.346	1.00	6.56	C
ATOM	6052	N	GLN	H	65	5.218	11.357	66.747	1.00	16.31	N
ATOM	6053	CA	GLN	H	65	5.896	10.171	66.233	1.00	15.36	C
ATOM	6054	C	GLN	H	65	5.728	10.090	64.721	1.00	13.38	C
ATOM	6055	O	GLN	H	65	4.608	10.124	64.198	1.00	11.85	O
ATOM	6056	CB	GLN	H	65	5.337	8.908	66.909	1.00	16.10	C
ATOM	6057	CG	GLN	H	65	5.923	7.570	66.411	1.00	17.28	C
ATOM	6058	CD	GLN	H	65	7.381	7.347	66.814	1.00	17.41	C
ATOM	6059	OE1	GLN	H	65	8.224	7.026	65.981	1.00	16.73	O
ATOM	6060	NE2	GLN	H	65	7.674	7.494	68.096	1.00	18.80	N
ATOM	6061	N	GLY	H	66	6.857	10.010	64.034	1.00	11.47	N
ATOM	6062	CA	GLY	H	66	6.844	9.935	62.595	1.00	12.23	C
ATOM	6063	C	GLY	H	66	7.432	11.182	61.969	1.00	12.71	C
ATOM	6064	O	GLY	H	66	8.208	11.087	61.007	1.00	13.79	O
ATOM	6065	N	ARG	H	67	7.103	12.349	62.526	1.00	12.38	N
ATOM	6066	CA	ARG	H	67	7.597	13.616	61.984	1.00	11.52	C
ATOM	6067	C	ARG	H	67	8.486	14.424	62.917	1.00	10.81	C
ATOM	6068	O	ARG	H	67	8.722	15.590	62.681	1.00	12.32	O

FIG. 53-94

ATOM	6070	CG	ARG	H	67	5.580	14.954	62.680	1.00	11.31	C
ATOM	6071	CD	ARG	H	67	4.372	15.659	62.146	1.00	11.22	C
ATOM	6072	NE	ARG	H	67	3.681	16.411	63.183	1.00	12.42	N
ATOM	6073	CZ	ARG	H	67	3.766	17.725	63.311	1.00	11.37	C
ATOM	6074	NH1	ARG	H	67	4.518	18.420	62.470	1.00	13.94	N
ATOM	6075	NH2	ARG	H	67	3.065	18.348	64.238	1.00	11.68	N
ATOM	6076	N	VAL	H	68	8.979	13.790	63.966	1.00	10.98	N
ATOM	6077	CA	VAL	H	68	9.850	14.455	64.926	1.00	8.54	C
ATOM	6078	C	VAL	H	68	11.088	13.585	65.116	1.00	8.61	C
ATOM	6079	O	VAL	H	68	10.988	12.357	65.122	1.00	9.69	O
ATOM	6080	CB	VAL	H	68	9.145	14.626	66.266	1.00	4.87	C
ATOM	6081	CG1	VAL	H	68	8.779	13.279	66.823	1.00	3.96	C
ATOM	6082	CG2	VAL	H	68	10.031	15.385	67.213	1.00	2.00	C
ATOM	6083	N	THR	H	69	12.245	14.209	65.291	1.00	7.97	N
ATOM	6084	CA	THR	H	69	13.482	13.465	65.458	1.00	7.36	C
ATOM	6085	C	THR	H	69	14.488	14.174	66.356	1.00	7.00	C
ATOM	6086	O	THR	H	69	14.910	15.297	66.076	1.00	6.55	O
ATOM	6087	CB	THR	H	69	14.135	13.212	64.086	1.00	9.59	C
ATOM	6088	OG1	THR	H	69	13.221	12.481	63.250	1.00	9.97	O
ATOM	6089	CG2	THR	H	69	15.453	12.447	64.238	1.00	7.33	C
ATOM	6090	N	ILE	H	70	14.906	13.499	67.418	1.00	7.70	N
ATOM	6091	CA	ILE	H	70	15.882	14.084	68.330	1.00	8.61	C
ATOM	6092	C	ILE	H	70	17.187	13.297	68.226	1.00	8.12	C
ATOM	6093	O	ILE	H	70	17.174	12.079	68.104	1.00	7.33	O
ATOM	6094	CB	ILE	H	70	15.373	14.081	69.806	1.00	7.10	C
ATOM	6095	CG1	ILE	H	70	13.936	14.606	69.872	1.00	6.03	C
ATOM	6096	CG2	ILE	H	70	16.260	14.965	70.664	1.00	4.82	C
ATOM	6097	CD1	ILE	H	70	13.321	14.525	71.249	1.00	6.55	C
ATOM	6098	N	THR	H	71	18.301	14.016	68.188	1.00	9.35	N
ATOM	6099	CA	THR	H	71	19.626	13.410	68.111	1.00	9.64	C
ATOM	6100	C	THR	H	71	20.553	14.239	68.968	1.00	11.13	C
ATOM	6101	O	THR	H	71	20.283	15.414	69.223	1.00	12.66	O
ATOM	6102	CB	THR	H	71	20.199	13.389	66.666	1.00	9.37	C
ATOM	6103	OG1	THR	H	71	20.079	14.688	66.072	1.00	7.60	O
ATOM	6104	CG2	THR	H	71	19.494	12.343	65.807	1.00	8.15	C
ATOM	6105	N	ALA	H	72	21.626	13.621	69.440	1.00	12.83	N
ATOM	6106	CA	ALA	H	72	22.597	14.315	70.259	1.00	14.33	C
ATOM	6107	C	ALA	H	72	23.951	13.964	69.695	1.00	16.43	C
ATOM	6108	O	ALA	H	72	24.210	12.807	69.384	1.00	16.79	O
ATOM	6109	CB	ALA	H	72	22.493	13.871	71.700	1.00	14.21	C
ATOM	6110	N	ASP	H	73	24.752	14.981	69.410	1.00	19.82	N
ATOM	6111	CA	ASP	H	73	26.088	14.754	68.905	1.00	21.26	C
ATOM	6112	C	ASP	H	73	26.945	14.764	70.158	1.00	21.75	C
ATOM	6113	O	ASP	H	73	27.011	15.764	70.874	1.00	21.34	O
ATOM	6114	CB	ASP	H	73	26.512	15.862	67.936	1.00	21.84	C
ATOM	6115	CG	ASP	H	73	27.880	15.604	67.305	1.00	24.12	C
ATOM	6116	OD1	ASP	H	73	28.662	14.782	67.823	1.00	24.23	O
ATOM	6117	OD2	ASP	H	73	28.191	16.242	66.282	1.00	27.83	O
ATOM	6118	N	LYS	H	74	27.555	13.626	70.453	1.00	23.06	N
ATOM	6119	CA	LYS	H	74	28.386	13.500	71.635	1.00	25.10	C
ATOM	6120	C	LYS	H	74	29.732	14.223	71.520	1.00	26.71	C
ATOM	6121	O	LYS	H	74	30.392	14.461	72.535	1.00	28.49	O
ATOM	6122	CB	LYS	H	74	28.574	12.020	71.982	1.00	25.76	C
ATOM	6123	CG	LYS	H	74	28.442	11.718	73.470	1.00	26.80	C
ATOM	6124	CD	LYS	H	74	29.699	12.112	74.215	1.00	28.23	C
ATOM	6125	CE	LYS	H	74	29.376	12.712	75.568	1.00	27.87	C
ATOM	6126	NZ	LYS	H	74	30.622	13.097	76.280	1.00	25.28	N
ATOM	6127	N	SER	H	75	30.131	14.591	70.304	1.00	26.51	N
ATOM	6128	CA	SER	H	75	31.396	15.301	70.111	1.00	27.08	C
ATOM	6129	C	SER	H	75	31.239	16.817	70.237	1.00	26.42	C
ATOM	6130	O	SER	H	75	32.218	17.523	70.429	1.00	27.72	O
ATOM	6131	CB	SER	H	75	32.031	14.964	68.756	1.00	28.79	C
ATOM	6132	OG	SER	H	75	31.455	15.726	67.703	1.00	30.42	O
ATOM	6133	N	THR	H	76	30.023	17.328	70.087	1.00	25.32	N
ATOM	6134	CA	THR	H	76	29.804	18.765	70.207	1.00	25.03	C
ATOM	6135	C	THR	H	76	28.834	19.066	71.348	1.00	26.48	C
ATOM	6136	O	THR	H	76	28.349	20.197	71.482	1.00	28.52	O
ATOM	6137	CB	THR	H	76	29.230	19.374	68.900	1.00	24.27	C
ATOM	6138	OG1	THR	H	76	28.024	18.691	68.536	1.00	23.85	O
ATOM	6139	CG2	THR	H	76	30.220	19.278	67.762	1.00	25.04	C

FIG. 53-95

ATOM	6141	CA	SER	H	77	27.608	18.209	73.278	1.00	23.20	C
ATOM	6142	C	SER	H	77	26.383	18.961	72.789	1.00	21.34	C
ATOM	6143	O	SER	H	77	25.941	19.925	73.410	1.00	21.95	O
ATOM	6144	CB	SER	H	77	28.260	18.957	74.440	1.00	22.09	C
ATOM	6145	OG	SER	H	77	29.178	18.130	75.133	1.00	23.49	O
ATOM	6146	N	THR	H	78	25.839	18.523	71.666	1.00	18.26	N
ATOM	6147	CA	THR	H	78	24.691	19.206	71.115	1.00	17.69	C
ATOM	6148	C	THR	H	78	23.495	18.309	70.868	1.00	15.95	C
ATOM	6149	O	THR	H	78	23.613	17.251	70.242	1.00	16.03	O
ATOM	6150	CB	THR	H	78	25.063	19.913	69.800	1.00	19.01	C
ATOM	6151	OG1	THR	H	78	26.186	20.773	70.031	1.00	19.55	O
ATOM	6152	CG2	THR	H	78	23.887	20.744	69.285	1.00	16.29	C
ATOM	6153	N	VAL	H	79	22.349	18.728	71.386	1.00	12.40	N
ATOM	6154	CA	VAL	H	79	21.111	17.997	71.187	1.00	9.30	C
ATOM	6155	C	VAL	H	79	20.452	18.627	69.956	1.00	7.84	C
ATOM	6156	O	VAL	H	79	20.746	19.782	69.609	1.00	6.59	O
ATOM	6157	CB	VAL	H	79	20.202	18.142	72.411	1.00	10.45	C
ATOM	6158	CG1	VAL	H	79	18.923	17.318	72.238	1.00	8.32	C
ATOM	6159	CG2	VAL	H	79	20.967	17.723	73.664	1.00	10.05	C
ATOM	6160	N	TYR	H	80	19.580	17.882	69.287	1.00	5.53	N
ATOM	6161	CA	TYR	H	80	18.913	18.391	68.091	1.00	4.33	C
ATOM	6162	C	TYR	H	80	17.461	17.987	68.072	1.00	3.56	C
ATOM	6163	O	TYR	H	80	17.088	16.997	68.694	1.00	7.00	O
ATOM	6164	CB	TYR	H	80	19.573	17.835	66.822	1.00	2.98	C
ATOM	6165	CG	TYR	H	80	20.886	18.477	66.468	1.00	3.35	C
ATOM	6166	CD1	TYR	H	80	20.925	19.665	65.745	1.00	3.20	C
ATOM	6167	CD2	TYR	H	80	22.092	17.913	66.876	1.00	3.31	C
ATOM	6168	CE1	TYR	H	80	22.133	20.280	65.447	1.00	5.35	C
ATOM	6169	CE2	TYR	H	80	23.302	18.518	66.582	1.00	4.91	C
ATOM	6170	CZ	TYR	H	80	23.318	19.700	65.871	1.00	5.18	C
ATOM	6171	OH	TYR	H	80	24.518	20.321	65.623	1.00	6.56	O
ATOM	6172	N	LEU	H	81	16.651	18.743	67.340	1.00	2.64	N
ATOM	6173	CA	LEU	H	81	15.241	18.435	67.187	1.00	3.48	C
ATOM	6174	C	LEU	H	81	14.854	18.843	65.784	1.00	5.71	C
ATOM	6175	O	LEU	H	81	14.997	20.012	65.415	1.00	7.81	O
ATOM	6176	CB	LEU	H	81	14.387	19.202	68.194	1.00	2.00	C
ATOM	6177	CG	LEU	H	81	12.891	18.890	68.410	1.00	3.11	C
ATOM	6178	CD1	LEU	H	81	12.050	20.133	68.146	1.00	2.00	C
ATOM	6179	CD2	LEU	H	81	12.396	17.710	67.607	1.00	2.00	C
ATOM	6180	N	GLU	H	82	14.497	17.864	64.960	1.00	7.38	N
ATOM	6181	CA	GLU	H	82	14.051	18.172	63.614	1.00	10.06	C
ATOM	6182	C	GLU	H	82	12.577	17.895	63.614	1.00	9.49	C
ATOM	6183	O	GLU	H	82	12.145	16.879	64.139	1.00	9.65	O
ATOM	6184	CB	GLU	H	82	14.703	17.316	62.529	1.00	10.92	C
ATOM	6185	CG	GLU	H	82	14.310	17.832	61.144	1.00	14.26	C
ATOM	6186	CD	GLU	H	82	14.779	16.966	60.008	1.00	18.22	C
ATOM	6187	OE1	GLU	H	82	15.929	17.160	59.551	1.00	20.46	O
ATOM	6188	OE2	GLU	H	82	13.987	16.103	59.556	1.00	21.67	O
ATOM	6189	N	LEU	H	83	11.809	18.807	63.047	1.00	9.97	N
ATOM	6190	CA	LEU	H	83	10.373	18.647	62.980	1.00	10.94	C
ATOM	6191	C	LEU	H	83	10.020	18.862	61.515	1.00	12.02	C
ATOM	6192	O	LEU	H	83	10.289	19.925	60.941	1.00	12.61	O
ATOM	6193	CB	LEU	H	83	9.679	19.659	63.906	1.00	8.22	C
ATOM	6194	CG	LEU	H	83	8.282	19.331	64.438	1.00	3.41	C
ATOM	6195	CD1	LEU	H	83	7.239	19.664	63.423	1.00	4.50	C
ATOM	6196	CD2	LEU	H	83	8.206	17.876	64.798	1.00	2.00	C
ATOM	6197	N	ARG	H	84	9.515	17.806	60.885	1.00	12.66	N
ATOM	6198	CA	ARG	H	84	9.171	17.869	59.482	1.00	12.67	C
ATOM	6199	C	ARG	H	84	7.675	17.981	59.275	1.00	13.55	C
ATOM	6200	O	ARG	H	84	6.895	17.817	60.216	1.00	13.09	O
ATOM	6201	CB	ARG	H	84	9.756	16.664	58.743	1.00	13.20	C
ATOM	6202	CG	ARG	H	84	9.181	15.329	59.178	1.00	15.41	C
ATOM	6203	CD	ARG	H	84	10.118	14.207	58.780	1.00	13.44	C
ATOM	6204	NE	ARG	H	84	11.392	14.347	59.483	1.00	10.62	N
ATOM	6205	CZ	ARG	H	84	11.758	13.614	60.529	1.00	6.51	C
ATOM	6206	NH1	ARG	H	84	10.950	12.664	61.005	1.00	3.06	N
ATOM	6207	NH2	ARG	H	84	12.921	13.870	61.115	1.00	2.00	N
ATOM	6208	N	ASN	H	85	7.292	18.278	58.035	1.00	14.44	N
ATOM	6209	CA	ASN	H	85	5.901	18.462	57.656	1.00	15.43	C
ATOM	6210	C	ASN	H	85	5.279	19.546	58.536	1.00	16.34	C

FIG. 53-96

ATOM	6212	CB	ASN	H	85	5.132	17.143	57.732	1.00	17.57	C
ATOM	6213	CG	ASN	H	85	5.594	16.141	56.681	1.00	18.99	C
ATOM	6214	OD1	ASN	H	85	5.725	14.944	56.952	1.00	17.64	O
ATOM	6215	ND2	ASN	H	85	5.854	16.631	55.476	1.00	18.85	N
ATOM	6216	N	LEU	H	86	6.010	20.651	58.663	1.00	16.01	N
ATOM	6217	CA	LEU	H	86	5.559	21.769	59.471	1.00	16.50	C
ATOM	6218	C	LEU	H	86	4.161	22.225	59.124	1.00	17.21	C
ATOM	6219	O	LEU	H	86	3.823	22.425	57.950	1.00	18.15	O
ATOM	6220	CB	LEU	H	86	6.524	22.947	59.375	1.00	14.51	C
ATOM	6221	CG	LEU	H	86	7.736	22.824	60.297	1.00	14.88	C
ATOM	6222	CD1	LEU	H	86	8.742	23.907	59.985	1.00	14.47	C
ATOM	6223	CD2	LEU	H	86	7.300	22.896	61.750	1.00	13.40	C
ATOM	6224	N	ARG	H	87	3.324	22.262	60.152	1.00	17.78	N
ATOM	6225	CA	ARG	H	87	1.947	22.715	60.049	1.00	15.84	C
ATOM	6226	C	ARG	H	87	1.994	24.080	60.733	1.00	13.95	C
ATOM	6227	O	ARG	H	87	2.875	24.334	61.560	1.00	11.95	O
ATOM	6228	CB	ARG	H	87	1.026	21.761	60.821	1.00	17.40	C
ATOM	6229	CG	ARG	H	87	0.758	20.438	60.123	1.00	21.87	C
ATOM	6230	CD	ARG	H	87	-0.359	20.572	59.089	1.00	26.43	C
ATOM	6231	NE	ARG	H	87	-0.135	19.781	57.874	1.00	31.72	N
ATOM	6232	CZ	ARG	H	87	0.788	20.057	56.946	1.00	32.88	C
ATOM	6233	NH1	ARG	H	87	1.588	21.114	57.086	1.00	33.85	N
ATOM	6234	NH2	ARG	H	87	0.922	19.267	55.885	1.00	32.25	N
ATOM	6235	N	SER	H	88	1.074	24.968	60.387	1.00	13.21	N
ATOM	6236	CA	SER	H	88	1.070	26.279	61.007	1.00	14.50	C
ATOM	6237	C	SER	H	88	0.905	26.139	62.522	1.00	14.12	C
ATOM	6238	O	SER	H	88	1.407	26.963	63.294	1.00	14.71	O
ATOM	6239	CB	SER	H	88	-0.029	27.164	60.409	1.00	14.65	C
ATOM	6240	OG	SER	H	88	-1.321	26.691	60.735	1.00	16.47	O
ATOM	6241	N	ASP	H	89	0.250	25.068	62.956	1.00	13.49	N
ATOM	6242	CA	ASP	H	89	0.049	24.857	64.384	1.00	12.51	C
ATOM	6243	C	ASP	H	89	1.309	24.452	65.138	1.00	11.36	C
ATOM	6244	O	ASP	H	89	1.308	24.407	66.369	1.00	12.92	O
ATOM	6245	CB	ASP	H	89	-1.090	23.876	64.644	1.00	12.20	C
ATOM	6246	CG	ASP	H	89	-0.900	22.576	63.947	1.00	10.88	C
ATOM	6247	OD1	ASP	H	89	-1.299	22.485	62.765	1.00	10.68	O
ATOM	6248	OD2	ASP	H	89	-0.359	21.651	64.581	1.00	7.76	O
ATOM	6249	N	ASP	H	90	2.395	24.202	64.414	1.00	10.72	N
ATOM	6250	CA	ASP	H	90	3.653	23.847	65.057	1.00	10.33	C
ATOM	6251	C	ASP	H	90	4.378	25.114	65.527	1.00	10.46	C
ATOM	6252	O	ASP	H	90	5.488	25.043	66.053	1.00	11.49	O
ATOM	6253	CB	ASP	H	90	4.549	23.027	64.118	1.00	10.98	C
ATOM	6254	CG	ASP	H	90	4.062	21.573	63.931	1.00	12.18	C
ATOM	6255	OD1	ASP	H	90	3.655	20.904	64.910	1.00	7.09	O
ATOM	6256	OD2	ASP	H	90	4.104	21.076	62.785	1.00	14.56	O
ATOM	6257	N	THR	H	91	3.750	26.272	65.319	1.00	10.54	N
ATOM	6258	CA	THR	H	91	4.299	27.569	65.725	1.00	9.98	C
ATOM	6259	C	THR	H	91	4.365	27.650	67.251	1.00	9.59	C
ATOM	6260	O	THR	H	91	3.334	27.785	67.924	1.00	8.95	O
ATOM	6261	CB	THR	H	91	3.414	28.730	65.238	1.00	10.45	C
ATOM	6262	OG1	THR	H	91	3.290	28.696	63.811	1.00	12.36	O
ATOM	6263	CG2	THR	H	91	4.030	30.053	65.637	1.00	12.42	C
ATOM	6264	N	ALA	H	92	5.573	27.611	67.795	1.00	9.83	N
ATOM	6265	CA	ALA	H	92	5.729	27.654	69.233	1.00	9.74	C
ATOM	6266	C	ALA	H	92	7.170	27.879	69.619	1.00	9.44	C
ATOM	6267	O	ALA	H	92	8.038	28.029	68.763	1.00	11.18	O
ATOM	6268	CB	ALA	H	92	5.242	26.355	69.833	1.00	12.61	C
ATOM	6269	N	VAL	H	93	7.414	27.898	70.922	1.00	8.45	N
ATOM	6270	CA	VAL	H	93	8.747	28.094	71.469	1.00	6.72	C
ATOM	6271	C	VAL	H	93	9.235	26.723	71.924	1.00	7.96	C
ATOM	6272	O	VAL	H	93	8.584	26.053	72.728	1.00	7.93	O
ATOM	6273	CB	VAL	H	93	8.710	29.040	72.658	1.00	3.48	C
ATOM	6274	CG1	VAL	H	93	10.101	29.382	73.094	1.00	4.97	C
ATOM	6275	CG2	VAL	H	93	7.954	30.286	72.300	1.00	2.20	C
ATOM	6276	N	TYR	H	94	10.373	26.309	71.379	1.00	8.12	N
ATOM	6277	CA	TYR	H	94	10.956	25.013	71.674	1.00	7.75	C
ATOM	6278	C	TYR	H	94	12.116	25.055	72.665	1.00	6.30	C
ATOM	6279	O	TYR	H	94	13.185	25.602	72.370	1.00	2.95	O
ATOM	6280	CB	TYR	H	94	11.385	24.340	70.361	1.00	11.44	C
ATOM	6281	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

FIG. 53-97

ATOM	6283	CD2	TYR	H	94	10.127	22.750	68.829	1.00	14.37	C
ATOM	6284	CE1	TYR	H	94	8.045	24.561	68.499	1.00	16.79	C
ATOM	6285	CE2	TYR	H	94	9.013	22.408	68.049	1.00	14.35	C
ATOM	6286	CZ	TYR	H	94	7.972	23.315	67.898	1.00	14.14	C
ATOM	6287	OH	TYR	H	94	6.827	22.958	67.221	1.00	11.38	O
ATOM	6288	N	PHE	H	95	11.881	24.502	73.853	1.00	6.46	N
ATOM	6289	CA	PHE	H	95	12.901	24.441	74.894	1.00	6.88	C
ATOM	6290	C	PHE	H	95	13.543	23.067	74.917	1.00	7.73	C
ATOM	6291	O	PHE	H	95	12.877	22.065	74.644	1.00	6.89	O
ATOM	6292	CB	PHE	H	95	12.291	24.626	76.284	1.00	4.64	C
ATOM	6293	CG	PHE	H	95	11.514	25.884	76.453	1.00	4.70	C
ATOM	6294	CD1	PHE	H	95	12.167	27.095	76.684	1.00	4.65	C
ATOM	6295	CD2	PHE	H	95	10.130	25.861	76.430	1.00	2.33	C
ATOM	6296	CE1	PHE	H	95	11.456	28.253	76.891	1.00	2.34	C
ATOM	6297	CE2	PHE	H	95	9.408	27.020	76.637	1.00	4.85	C
ATOM	6298	CZ	PHE	H	95	10.076	28.225	76.870	1.00	3.13	C
ATOM	6299	N	CYS	H	96	14.835	23.024	75.214	1.00	8.72	N
ATOM	6300	CA	CYS	H	96	15.523	21.757	75.382	1.00	10.25	C
ATOM	6301	C	CYS	H	96	15.733	21.734	76.894	1.00	10.64	C
ATOM	6302	O	CYS	H	96	15.935	22.790	77.513	1.00	11.69	O
ATOM	6303	CB	CYS	H	96	16.865	21.720	74.640	1.00	11.55	C
ATOM	6304	SG	CYS	H	96	18.050	23.018	75.110	1.00	17.70	S
ATOM	6305	N	ALA	H	97	15.621	20.566	77.510	1.00	9.40	N
ATOM	6306	CA	ALA	H	97	15.806	20.475	78.954	1.00	7.79	C
ATOM	6307	C	ALA	H	97	16.595	19.227	79.279	1.00	7.44	C
ATOM	6308	O	ALA	H	97	16.989	18.494	78.384	1.00	8.41	O
ATOM	6309	CB	ALA	H	97	14.459	20.451	79.653	1.00	7.01	C
ATOM	6310	N	GLY	H	98	16.837	18.990	80.558	1.00	8.12	N
ATOM	6311	CA	GLY	H	98	17.578	17.811	80.946	1.00	7.91	C
ATOM	6312	C	GLY	H	98	17.827	17.679	82.427	1.00	7.80	C
ATOM	6313	O	GLY	H	98	17.630	18.621	83.202	1.00	7.39	O
ATOM	6314	N	VAL	H	99	18.168	16.457	82.823	1.00	9.74	N
ATOM	6315	CA	VAL	H	99	18.501	16.113	84.201	1.00	11.02	C
ATOM	6316	C	VAL	H	99	19.730	15.240	84.106	1.00	11.60	C
ATOM	6317	O	VAL	H	99	20.126	14.821	83.022	1.00	13.99	O
ATOM	6318	CB	VAL	H	99	17.412	15.290	84.919	1.00	10.75	C
ATOM	6319	CG1	VAL	H	99	16.259	16.173	85.304	1.00	11.64	C
ATOM	6320	CG2	VAL	H	99	16.948	14.135	84.040	1.00	13.26	C
ATOM	6321	N	TYR	H	100	20.325	14.957	85.249	1.00	11.05	N
ATOM	6322	CA	TYR	H	100	21.518	14.138	85.318	1.00	7.98	C
ATOM	6323	C	TYR	H	100	21.123	12.763	85.824	1.00	6.09	C
ATOM	6324	O	TYR	H	100	20.302	12.654	86.737	1.00	4.87	O
ATOM	6325	CB	TYR	H	100	22.515	14.817	86.256	1.00	7.21	C
ATOM	6326	CG	TYR	H	100	23.632	13.960	86.746	1.00	3.12	C
ATOM	6327	CD1	TYR	H	100	23.466	13.151	87.861	1.00	2.00	C
ATOM	6328	CD2	TYR	H	100	24.868	13.988	86.123	1.00	3.75	C
ATOM	6329	CE1	TYR	H	100	24.498	12.396	88.344	1.00	2.00	C
ATOM	6330	CE2	TYR	H	100	25.923	13.224	86.600	1.00	4.79	C
ATOM	6331	CZ	TYR	H	100	25.731	12.433	87.716	1.00	2.60	C
ATOM	6332	OH	TYR	H	100	26.779	11.707	88.207	1.00	4.31	O
ATOM	6333	N	GLU	H	101	21.690	11.736	85.194	1.00	6.38	N
ATOM	6334	CA	GLU	H	101	21.441	10.328	85.519	1.00	6.30	C
ATOM	6335	C	GLU	H	101	22.628	9.741	86.301	1.00	7.29	C
ATOM	6336	O	GLU	H	101	22.465	9.282	87.423	1.00	6.15	O
ATOM	6337	CB	GLU	H	101	21.221	9.531	84.223	1.00	5.89	C
ATOM	6338	CG	GLU	H	101	20.277	10.174	83.187	1.00	3.98	C
ATOM	6339	CD	GLU	H	101	18.800	10.099	83.563	1.00	5.47	C
ATOM	6340	OE1	GLU	H	101	18.494	9.684	84.697	1.00	7.08	O
ATOM	6341	OE2	GLU	H	101	17.929	10.455	82.733	1.00	2.69	O
ATOM	6342	N	GLY	H	102	23.821	9.752	85.706	1.00	9.60	N
ATOM	6343	CA	GLY	H	102	24.995	9.237	86.395	1.00	12.31	C
ATOM	6344	C	GLY	H	102	25.905	8.258	85.666	1.00	16.39	C
ATOM	6345	O	GLY	H	102	26.983	7.950	86.165	1.00	15.66	O
ATOM	6346	N	GLU	H	103	25.496	7.817	84.479	1.00	20.62	N
ATOM	6347	CA	GLU	H	103	26.242	6.845	83.673	1.00	24.85	C
ATOM	6348	C	GLU	H	103	27.737	7.113	83.447	1.00	27.34	C
ATOM	6349	O	GLU	H	103	28.505	7.076	84.399	1.00	30.02	O
ATOM	6350	CB	GLU	H	103	25.477	6.583	82.367	1.00	26.05	C
ATOM	6351	CG	GLU	H	103	26.151	5.678	81.326	1.00	30.53	C
ATOM	6352	CD	GLU	H	103	26.767	4.408	81.883	1.00	31.41	C

FIG. 53-98

ATOM	6354	OE2	GLU	H	103	26.113	3.348	81.832	1.00	33.96	O
ATOM	6355	N	ALA	H	104	28.159	7.362	82.209	1.00	29.27	N
ATOM	6356	CA	ALA	H	104	29.570	7.599	81.886	1.00	30.55	C
ATOM	6357	C	ALA	H	104	30.494	6.499	82.400	1.00	30.87	C
ATOM	6358	O	ALA	H	104	31.388	6.757	83.213	1.00	30.76	O
ATOM	6359	CB	ALA	H	104	30.025	8.954	82.407	1.00	30.95	C
ATOM	6360	N	ASP	H	105	30.291	5.291	81.881	1.00	32.13	N
ATOM	6361	CA	ASP	H	105	31.063	4.104	82.241	1.00	33.17	C
ATOM	6362	C	ASP	H	105	31.007	3.834	83.736	1.00	33.82	C
ATOM	6363	O	ASP	H	105	32.013	3.875	84.455	1.00	36.41	O
ATOM	6364	CB	ASP	H	105	32.508	4.184	81.730	1.00	34.46	C
ATOM	6365	CG	ASP	H	105	32.600	4.150	80.203	1.00	36.30	C
ATOM	6366	OD1	ASP	H	105	31.555	4.016	79.521	1.00	36.30	O
ATOM	6367	OD2	ASP	H	105	33.726	4.281	79.676	1.00	36.00	O
ATOM	6368	N	GLU	H	106	29.788	3.602	84.197	1.00	31.59	N
ATOM	6369	CA	GLU	H	106	29.494	3.287	85.585	1.00	27.78	C
ATOM	6370	C	GLU	H	106	28.275	2.369	85.548	1.00	25.32	C
ATOM	6371	O	GLU	H	106	28.024	1.627	86.499	1.00	26.26	O
ATOM	6372	CB	GLU	H	106	29.161	4.549	86.383	1.00	27.49	C
ATOM	6373	CG	GLU	H	106	30.310	5.517	86.575	1.00	27.59	C
ATOM	6374	CD	GLU	H	106	29.980	6.606	87.582	1.00	27.57	C
ATOM	6375	OE1	GLU	H	106	29.898	6.304	88.790	1.00	28.56	O
ATOM	6376	OE2	GLU	H	106	29.817	7.767	87.185	1.00	24.49	O
ATOM	6377	N	GLY	H	107	27.521	2.438	84.451	1.00	21.84	N
ATOM	6378	CA	GLY	H	107	26.343	1.613	84.275	1.00	18.93	C
ATOM	6379	C	GLY	H	107	25.117	2.132	84.991	1.00	18.22	C
ATOM	6380	O	GLY	H	107	24.013	1.655	84.735	1.00	17.35	O
ATOM	6381	N	GLU	H	108	25.311	3.087	85.901	1.00	18.06	N
ATOM	6382	CA	GLU	H	108	24.218	3.674	86.681	1.00	16.77	C
ATOM	6383	C	GLU	H	108	23.404	4.632	85.816	1.00	15.01	C
ATOM	6384	O	GLU	H	108	23.962	5.403	85.041	1.00	15.22	O
ATOM	6385	CB	GLU	H	108	24.778	4.403	87.901	1.00	17.99	C
ATOM	6386	CG	GLU	H	108	23.715	4.903	88.859	1.00	19.84	C
ATOM	6387	CD	GLU	H	108	24.290	5.769	89.948	1.00	20.33	C
ATOM	6388	OE1	GLU	H	108	24.510	6.964	89.685	1.00	22.12	O
ATOM	6389	OE2	GLU	H	108	24.545	5.262	91.062	1.00	20.70	O
ATOM	6390	N	TYR	H	109	22.090	4.612	85.981	1.00	13.44	N
ATOM	6391	CA	TYR	H	109	21.216	5.438	85.170	1.00	13.22	C
ATOM	6392	C	TYR	H	109	19.809	5.411	85.753	1.00	13.74	C
ATOM	6393	O	TYR	H	109	19.050	4.471	85.510	1.00	14.84	O
ATOM	6394	CB	TYR	H	109	21.198	4.877	83.745	1.00	13.35	C
ATOM	6395	CG	TYR	H	109	20.833	5.877	82.692	1.00	13.43	C
ATOM	6396	CD1	TYR	H	109	21.780	6.772	82.204	1.00	15.22	C
ATOM	6397	CD2	TYR	H	109	19.528	5.976	82.223	1.00	14.92	C
ATOM	6398	CE1	TYR	H	109	21.433	7.753	81.275	1.00	15.72	C
ATOM	6399	CE2	TYR	H	109	19.170	6.950	81.296	1.00	15.14	C
ATOM	6400	CZ	TYR	H	109	20.127	7.837	80.833	1.00	15.74	C
ATOM	6401	OH	TYR	H	109	19.764	8.826	79.955	1.00	18.81	O
ATOM	6402	N	ASP	H	110	19.461	6.455	86.499	1.00	14.02	N
ATOM	6403	CA	ASP	H	110	18.150	6.568	87.141	1.00	14.21	C
ATOM	6404	C	ASP	H	110	16.998	6.584	86.153	1.00	12.92	C
ATOM	6405	O	ASP	H	110	15.931	6.034	86.421	1.00	12.58	O
ATOM	6406	CB	ASP	H	110	18.058	7.871	87.948	1.00	17.79	C
ATOM	6407	CG	ASP	H	110	18.872	7.852	89.221	1.00	23.07	C
ATOM	6408	OD1	ASP	H	110	19.909	7.160	89.272	1.00	26.33	O
ATOM	6409	OD2	ASP	H	110	18.481	8.567	90.173	1.00	25.02	O
ATOM	6410	N	ASN	H	111	17.222	7.267	85.031	1.00	12.61	N
ATOM	6411	CA	ASN	H	111	16.232	7.479	83.978	1.00	10.59	C
ATOM	6412	C	ASN	H	111	15.194	8.448	84.542	1.00	9.97	C
ATOM	6413	O	ASN	H	111	13.989	8.220	84.436	1.00	10.86	O
ATOM	6414	CB	ASN	H	111	15.564	6.183	83.529	1.00	11.03	C
ATOM	6415	CG	ASN	H	111	15.239	6.188	82.034	1.00	16.38	C
ATOM	6416	OD1	ASN	H	111	14.630	7.129	81.510	1.00	17.18	O
ATOM	6417	ND2	ASN	H	111	15.683	5.153	81.333	1.00	17.14	N
ATOM	6418	N	ASN	H	112	15.676	9.530	85.153	1.00	8.07	N
ATOM	6419	CA	ASN	H	112	14.813	10.549	85.756	1.00	7.55	C
ATOM	6420	C	ASN	H	112	13.951	11.218	84.688	1.00	7.89	C
ATOM	6421	O	ASN	H	112	14.464	11.811	83.737	1.00	8.98	O
ATOM	6422	CB	ASN	H	112	15.644	11.632	86.462	1.00	5.99	C
ATOM	6423	CG	ASN	H	112	16.641	11.067	87.462	1.00	5.32	C

FIG. 53-99

ATOM	6425	ND2	ASN	H	112	17.921	11.173	87.148	1.00	2.00	N
ATOM	6426	N	GLY	H	113	12.639	11.153	84.863	1.00	9.15	N
ATOM	6427	CA	GLY	H	113	11.733	11.765	83.907	1.00	9.70	C
ATOM	6428	C	GLY	H	113	11.526	13.268	84.031	1.00	9.37	C
ATOM	6429	O	GLY	H	113	11.079	13.898	83.079	1.00	10.86	O
ATOM	6430	N	PHE	H	114	11.822	13.851	85.189	1.00	9.22	N
ATOM	6431	CA	PHE	H	114	11.626	15.292	85.372	1.00	8.10	C
ATOM	6432	C	PHE	H	114	12.732	16.074	84.653	1.00	8.34	C
ATOM	6433	O	PHE	H	114	13.664	15.467	84.105	1.00	9.11	O
ATOM	6434	CB	PHE	H	114	11.533	15.660	86.872	1.00	6.12	C
ATOM	6435	CG	PHE	H	114	12.770	15.328	87.662	1.00	4.82	C
ATOM	6436	CD1	PHE	H	114	12.910	14.076	88.261	1.00	2.00	C
ATOM	6437	CD2	PHE	H	114	13.805	16.256	87.789	1.00	2.00	C
ATOM	6438	CE1	PHE	H	114	14.060	13.743	88.974	1.00	2.00	C
ATOM	6439	CE2	PHE	H	114	14.959	15.932	88.499	1.00	4.28	C
ATOM	6440	CZ	PHE	H	114	15.085	14.661	89.098	1.00	2.99	C
ATOM	6441	N	LEU	H	115	12.643	17.408	84.677	1.00	6.85	N
ATOM	6442	CA	LEU	H	115	13.607	18.272	84.000	1.00	5.32	C
ATOM	6443	C	LEU	H	115	14.176	19.366	84.918	1.00	6.67	C
ATOM	6444	O	LEU	H	115	13.459	20.266	85.360	1.00	7.52	O
ATOM	6445	CB	LEU	H	115	12.930	18.899	82.792	1.00	3.62	C
ATOM	6446	CG	LEU	H	115	12.123	17.922	81.946	1.00	2.00	C
ATOM	6447	CD1	LEU	H	115	10.991	18.632	81.234	1.00	2.33	C
ATOM	6448	CD2	LEU	H	115	13.041	17.237	80.971	1.00	4.15	C
ATOM	6449	N	LYS	H	116	15.490	19.318	85.124	1.00	7.90	N
ATOM	6450	CA	LYS	H	116	16.214	20.236	86.000	1.00	8.29	C
ATOM	6451	C	LYS	H	116	16.742	21.483	85.307	1.00	8.65	C
ATOM	6452	O	LYS	H	116	16.731	22.571	85.887	1.00	6.26	O
ATOM	6453	CB	LYS	H	116	17.387	19.486	86.640	1.00	8.77	C
ATOM	6454	CG	LYS	H	116	18.337	20.313	87.510	1.00	9.73	C
ATOM	6455	CD	LYS	H	116	17.703	20.766	88.803	1.00	10.23	C
ATOM	6456	CE	LYS	H	116	18.755	21.216	89.822	1.00	13.09	C
ATOM	6457	NZ	LYS	H	116	19.257	20.107	90.704	1.00	11.05	N
ATOM	6458	N	HIS	H	117	17.290	21.302	84.108	1.00	9.62	N
ATOM	6459	CA	HIS	H	117	17.847	22.414	83.349	1.00	9.20	C
ATOM	6460	C	HIS	H	117	17.001	22.697	82.124	1.00	8.69	C
ATOM	6461	O	HIS	H	117	16.453	21.787	81.524	1.00	9.06	O
ATOM	6462	CB	HIS	H	117	19.285	22.112	82.931	1.00	9.50	C
ATOM	6463	CG	HIS	H	117	20.171	21.707	84.069	1.00	13.01	C
ATOM	6464	ND1	HIS	H	117	20.574	22.552	85.080	1.00	14.89	N
ATOM	6465	CD2	HIS	H	117	20.713	20.499	84.367	1.00	12.49	C
ATOM	6466	CE1	HIS	H	117	21.323	21.847	85.936	1.00	12.68	C
ATOM	6467	NE2	HIS	H	117	21.438	20.592	85.545	1.00	13.22	N
ATOM	6468	N	TRP	H	118	16.882	23.968	81.768	1.00	8.39	N
ATOM	6469	CA	TRP	H	118	16.108	24.359	80.600	1.00	7.76	C
ATOM	6470	C	TRP	H	118	16.898	25.347	79.740	1.00	6.56	C
ATOM	6471	O	TRP	H	118	17.981	25.784	80.128	1.00	5.39	O
ATOM	6472	CB	TRP	H	118	14.781	24.983	81.027	1.00	7.76	C
ATOM	6473	CG	TRP	H	118	13.827	24.030	81.689	1.00	3.56	C
ATOM	6474	CD1	TRP	H	118	13.903	23.539	82.953	1.00	4.13	C
ATOM	6475	CD2	TRP	H	118	12.601	23.535	81.143	1.00	2.00	C
ATOM	6476	NE1	TRP	H	118	12.794	22.782	83.240	1.00	2.00	N
ATOM	6477	CE2	TRP	H	118	11.980	22.766	82.144	1.00	2.00	C
ATOM	6478	CE3	TRP	H	118	11.967	23.674	79.909	1.00	2.00	C
ATOM	6479	CZ2	TRP	H	118	10.753	22.141	81.946	1.00	3.79	C
ATOM	6480	CZ3	TRP	H	118	10.756	23.053	79.715	1.00	2.00	C
ATOM	6481	CH2	TRP	H	118	10.158	22.296	80.728	1.00	2.64	C
ATOM	6482	N	GLY	H	119	16.374	25.655	78.559	1.00	6.44	N
ATOM	6483	CA	GLY	H	119	17.035	26.585	77.664	1.00	7.62	C
ATOM	6484	C	GLY	H	119	16.254	27.879	77.536	1.00	8.65	C
ATOM	6485	O	GLY	H	119	15.098	27.949	77.953	1.00	10.48	O
ATOM	6486	N	GLN	H	120	16.876	28.909	76.963	1.00	10.80	N
ATOM	6487	CA	GLN	H	120	16.216	30.214	76.798	1.00	10.30	C
ATOM	6488	C	GLN	H	120	14.976	30.124	75.931	1.00	8.85	C
ATOM	6489	O	GLN	H	120	14.055	30.929	76.079	1.00	9.21	O
ATOM	6490	CB	GLN	H	120	17.158	31.247	76.194	1.00	8.92	C
ATOM	6491	CG	GLN	H	120	17.334	31.102	74.704	1.00	10.45	C
ATOM	6492	CD	GLN	H	120	18.639	30.437	74.332	1.00	12.55	C
ATOM	6493	OE1	GLN	H	120	19.326	29.855	75.177	1.00	10.90	O
ATOM	6494	NE2	GLN	H	120	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	N

FIG. 53-100

ATOM	6496	CA	GLY	H	121	13.839	28.985	74.135	1.00	6.60	C
ATOM	6497	C	GLY	H	121	14.180	29.405	72.729	1.00	6.68	C
ATOM	6498	O	GLY	H	121	15.033	30.268	72.518	1.00	8.82	O
ATOM	6499	N	THR	H	122	13.547	28.757	71.763	1.00	5.74	N
ATOM	6500	CA	THR	H	122	13.766	29.059	70.369	1.00	6.29	C
ATOM	6501	C	THR	H	122	12.391	29.208	69.782	1.00	8.39	C
ATOM	6502	O	THR	H	122	11.602	28.262	69.818	1.00	11.50	O
ATOM	6503	CB	THR	H	122	14.463	27.900	69.679	1.00	6.38	C
ATOM	6504	OG1	THR	H	122	15.664	27.599	70.382	1.00	11.11	O
ATOM	6505	CG2	THR	H	122	14.813	28.245	68.261	1.00	4.29	C
ATOM	6506	N	LEU	H	123	12.048	30.411	69.336	1.00	7.48	N
ATOM	6507	CA	LEU	H	123	10.735	30.592	68.740	1.00	7.17	C
ATOM	6508	C	LEU	H	123	10.799	30.123	67.302	1.00	6.63	C
ATOM	6509	O	LEU	H	123	11.748	30.442	66.584	1.00	6.20	O
ATOM	6510	CB	LEU	H	123	10.277	32.045	68.765	1.00	6.20	C
ATOM	6511	CG	LEU	H	123	8.911	32.153	68.087	1.00	5.67	C
ATOM	6512	CD1	LEU	H	123	7.887	31.381	68.902	1.00	2.00	C
ATOM	6513	CD2	LEU	H	123	8.505	33.612	67.928	1.00	8.02	C
ATOM	6514	N	VAL	H	124	9.814	29.318	66.917	1.00	6.22	N
ATOM	6515	CA	VAL	H	124	9.710	28.801	65.566	1.00	4.41	C
ATOM	6516	C	VAL	H	124	8.327	29.187	65.103	1.00	5.26	C
ATOM	6517	O	VAL	H	124	7.327	28.713	65.655	1.00	4.50	O
ATOM	6518	CB	VAL	H	124	9.825	27.266	65.510	1.00	3.42	C
ATOM	6519	CG1	VAL	H	124	9.580	26.778	64.091	1.00	4.69	C
ATOM	6520	CG2	VAL	H	124	11.200	26.810	65.978	1.00	2.89	C
ATOM	6521	N	THR	H	125	8.269	30.095	64.134	1.00	5.24	N
ATOM	6522	CA	THR	H	125	6.997	30.547	63.591	1.00	5.65	C
ATOM	6523	C	THR	H	125	6.866	29.888	62.233	1.00	5.34	C
ATOM	6524	O	THR	H	125	7.829	29.869	61.453	1.00	3.74	O
ATOM	6525	CB	THR	H	125	6.963	32.081	63.363	1.00	5.97	C
ATOM	6526	OG1	THR	H	125	7.710	32.750	64.386	1.00	8.20	O
ATOM	6527	CG2	THR	H	125	5.522	32.572	63.410	1.00	5.65	C
ATOM	6528	N	VAL	H	126	5.692	29.327	61.967	1.00	4.89	N
ATOM	6529	CA	VAL	H	126	5.441	28.672	60.700	1.00	5.00	C
ATOM	6530	C	VAL	H	126	4.238	29.367	60.101	1.00	5.63	C
ATOM	6531	O	VAL	H	126	3.140	29.301	60.662	1.00	4.20	O
ATOM	6532	CB	VAL	H	126	5.143	27.175	60.890	1.00	5.78	C
ATOM	6533	CG1	VAL	H	126	5.045	26.490	59.529	1.00	5.45	C
ATOM	6534	CG2	VAL	H	126	6.234	26.513	61.760	1.00	4.07	C
ATOM	6535	N	THR	H	127	4.450	30.067	58.987	1.00	7.29	N
ATOM	6536	CA	THR	H	127	3.377	30.813	58.334	1.00	10.19	C
ATOM	6537	C	THR	H	127	3.686	31.061	56.867	1.00	11.09	C
ATOM	6538	O	THR	H	127	4.841	31.325	56.496	1.00	11.77	O
ATOM	6539	CB	THR	H	127	3.193	32.237	58.947	1.00	11.86	C
ATOM	6540	OG1	THR	H	127	3.308	32.192	60.375	1.00	18.89	O
ATOM	6541	CG2	THR	H	127	1.830	32.821	58.576	1.00	11.36	C
ATOM	6542	N	SER	H	128	2.622	31.078	56.065	1.00	10.84	N
ATOM	6543	CA	SER	H	128	2.690	31.339	54.634	1.00	10.37	C
ATOM	6544	C	SER	H	128	3.056	32.802	54.374	1.00	10.64	C
ATOM	6545	O	SER	H	128	3.520	33.139	53.292	1.00	11.41	O
ATOM	6546	CB	SER	H	128	1.333	31.054	54.017	1.00	11.13	C
ATOM	6547	OG	SER	H	128	0.312	31.613	54.834	1.00	12.99	O
ATOM	6548	N	ALA	H	129	2.834	33.664	55.364	1.00	11.65	N
ATOM	6549	CA	ALA	H	129	3.147	35.094	55.260	1.00	13.12	C
ATOM	6550	C	ALA	H	129	4.649	35.359	55.207	1.00	14.65	C
ATOM	6551	O	ALA	H	129	5.431	34.589	55.759	1.00	16.91	O
ATOM	6552	CB	ALA	H	129	2.540	35.841	56.420	1.00	11.97	C
ATOM	6553	N	SER	H	130	5.046	36.453	54.560	1.00	15.13	N
ATOM	6554	CA	SER	H	130	6.465	36.818	54.439	1.00	14.25	C
ATOM	6555	C	SER	H	130	6.849	37.928	55.413	1.00	12.80	C
ATOM	6556	O	SER	H	130	5.993	38.666	55.901	1.00	11.17	O
ATOM	6557	CB	SER	H	130	6.782	37.271	53.011	1.00	14.65	C
ATOM	6558	OG	SER	H	130	6.508	36.243	52.069	1.00	17.09	O
ATOM	6559	N	THR	H	131	8.142	38.052	55.678	1.00	12.55	N
ATOM	6560	CA	THR	H	131	8.659	39.067	56.598	1.00	14.01	C
ATOM	6561	C	THR	H	131	8.349	40.497	56.147	1.00	14.38	C
ATOM	6562	O	THR	H	131	8.318	40.796	54.944	1.00	14.04	O
ATOM	6563	CB	THR	H	131	10.195	38.919	56.769	1.00	14.47	C
ATOM	6564	OG1	THR	H	131	10.510	37.582	57.185	1.00	12.21	O
ATOM	6565	CG2	THR	H	131	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

FIG. 53-101

ATOM	6567	CA	LYS	H	132	7.823	42.770	56.819	1.00	15.47	C
ATOM	6568	C	LYS	H	132	7.781	43.637	58.072	1.00	16.55	C
ATOM	6569	O	LYS	H	132	7.291	43.205	59.139	1.00	17.63	O
ATOM	6570	CB	LYS	H	132	6.513	42.915	56.037	1.00	15.09	C
ATOM	6571	CG	LYS	H	132	5.242	42.780	56.850	1.00	16.23	C
ATOM	6572	CD	LYS	H	132	4.027	43.112	55.997	1.00	16.20	C
ATOM	6573	CE	LYS	H	132	4.057	44.551	55.500	1.00	16.81	C
ATOM	6574	NZ	LYS	H	132	3.995	45.539	56.630	1.00	21.10	N
ATOM	6575	N	GLY	H	133	8.348	44.837	57.947	1.00	15.20	N
ATOM	6576	CA	GLY	H	133	8.363	45.790	59.042	1.00	12.03	C
ATOM	6577	C	GLY	H	133	6.963	46.314	59.284	1.00	9.06	C
ATOM	6578	O	GLY	H	133	6.141	46.329	58.366	1.00	9.32	O
ATOM	6579	N	PRO	H	134	6.660	46.765	60.502	1.00	7.19	N
ATOM	6580	CA	PRO	H	134	5.326	47.273	60.806	1.00	7.38	C
ATOM	6581	C	PRO	H	134	5.055	48.719	60.416	1.00	8.86	C
ATOM	6582	O	PRO	H	134	5.958	49.476	60.028	1.00	7.17	O
ATOM	6583	CB	PRO	H	134	5.250	47.103	62.312	1.00	6.38	C
ATOM	6584	CG	PRO	H	134	6.640	47.479	62.730	1.00	6.33	C
ATOM	6585	CD	PRO	H	134	7.510	46.766	61.706	1.00	7.21	C
ATOM	6586	N	SER	H	135	3.778	49.075	60.529	1.00	10.15	N
ATOM	6587	CA	SER	H	135	3.281	50.404	60.252	1.00	9.30	C
ATOM	6588	C	SER	H	135	3.074	51.015	61.616	1.00	9.91	C
ATOM	6589	O	SER	H	135	2.216	50.569	62.373	1.00	10.72	O
ATOM	6590	CB	SER	H	135	1.927	50.333	59.545	1.00	9.06	C
ATOM	6591	OG	SER	H	135	2.054	49.874	58.212	1.00	12.48	O
ATOM	6592	N	VAL	H	136	3.903	51.983	61.964	1.00	10.98	N
ATOM	6593	CA	VAL	H	136	3.765	52.641	63.244	1.00	11.00	C
ATOM	6594	C	VAL	H	136	2.875	53.876	63.099	1.00	10.33	C
ATOM	6595	O	VAL	H	136	3.197	54.806	62.363	1.00	8.56	O
ATOM	6596	CB	VAL	H	136	5.136	53.037	63.814	1.00	13.40	C
ATOM	6597	CG1	VAL	H	136	4.974	53.698	65.193	1.00	13.53	C
ATOM	6598	CG2	VAL	H	136	6.029	51.803	63.905	1.00	14.01	C
ATOM	6599	N	PHE	H	137	1.733	53.843	63.776	1.00	11.17	N
ATOM	6600	CA	PHE	H	137	0.773	54.942	63.790	1.00	11.79	C
ATOM	6601	C	PHE	H	137	0.656	55.374	65.250	1.00	13.75	C
ATOM	6602	O	PHE	H	137	0.747	54.547	66.148	1.00	12.53	O
ATOM	6603	CB	PHE	H	137	-0.597	54.469	63.293	1.00	11.07	C
ATOM	6604	CG	PHE	H	137	-0.577	53.926	61.906	1.00	10.97	C
ATOM	6605	CD1	PHE	H	137	-0.157	54.723	60.840	1.00	12.08	C
ATOM	6606	CD2	PHE	H	137	-0.954	52.613	61.659	1.00	10.56	C
ATOM	6607	CE1	PHE	H	137	-0.112	54.215	59.545	1.00	10.06	C
ATOM	6608	CE2	PHE	H	137	-0.914	52.097	60.375	1.00	10.49	C
ATOM	6609	CZ	PHE	H	137	-0.493	52.898	59.316	1.00	10.89	C
ATOM	6610	N	PRO	H	138	0.458	56.676	65.507	1.00	15.89	N
ATOM	6611	CA	PRO	H	138	0.336	57.195	66.870	1.00	18.02	C
ATOM	6612	C	PRO	H	138	-1.116	57.271	67.323	1.00	20.61	C
ATOM	6613	O	PRO	H	138	-2.028	57.423	66.502	1.00	22.40	O
ATOM	6614	CB	PRO	H	138	0.915	58.588	66.728	1.00	17.19	C
ATOM	6615	CG	PRO	H	138	0.306	59.018	65.429	1.00	17.20	C
ATOM	6616	CD	PRO	H	138	0.434	57.780	64.532	1.00	16.18	C
ATOM	6617	N	LEU	H	139	-1.320	57.182	68.636	1.00	22.53	N
ATOM	6618	CA	LEU	H	139	-2.647	57.256	69.243	1.00	24.41	C
ATOM	6619	C	LEU	H	139	-2.765	58.622	69.912	1.00	26.20	C
ATOM	6620	O	LEU	H	139	-2.600	58.752	71.120	1.00	25.66	O
ATOM	6621	CB	LEU	H	139	-2.812	56.130	70.266	1.00	22.44	C
ATOM	6622	CG	LEU	H	139	-3.492	54.850	69.786	1.00	21.57	C
ATOM	6623	CD1	LEU	H	139	-3.350	54.682	68.286	1.00	21.35	C
ATOM	6624	CD2	LEU	H	139	-2.921	53.658	70.536	1.00	20.98	C
ATOM	6625	N	ALA	H	140	-2.990	59.640	69.089	1.00	30.01	N
ATOM	6626	CA	ALA	H	140	-3.104	61.027	69.534	1.00	31.42	C
ATOM	6627	C	ALA	H	140	-3.967	61.181	70.768	1.00	32.96	C
ATOM	6628	O	ALA	H	140	-5.041	60.575	70.865	1.00	32.60	O
ATOM	6629	CB	ALA	H	140	-3.643	61.908	68.399	1.00	31.26	C
ATOM	6630	N	PRO	H	141	-3.502	61.996	71.736	1.00	34.92	N
ATOM	6631	CA	PRO	H	141	-4.200	62.264	72.997	1.00	36.69	C
ATOM	6632	C	PRO	H	141	-5.699	62.466	72.814	1.00	38.82	C
ATOM	6633	O	PRO	H	141	-6.135	63.500	72.312	1.00	38.07	O
ATOM	6634	CB	PRO	H	141	-3.512	63.532	73.492	1.00	35.13	C
ATOM	6635	CG	PRO	H	141	-2.094	63.290	73.100	1.00	33.37	C
ATOM	6636	CD	PRO	H	141	-2.225	62.737	71.685	1.00	33.56	C

FIG. 53-102

ATOM	6638	CA	SER	H	142	-7.924	61.421	73.169	1.00	44.81	C
ATOM	6639	C	SER	H	142	-8.580	62.786	73.342	1.00	46.31	C
ATOM	6640	O	SER	H	142	-9.637	63.057	72.768	1.00	47.19	O
ATOM	6641	CB	SER	H	142	-8.463	60.442	74.214	1.00	45.28	C
ATOM	6642	OG	SER	H	142	-7.701	60.515	75.412	1.00	45.59	O
ATOM	6643	N	SER	H	143	-7.943	63.617	74.158	1.00	47.43	N
ATOM	6644	CA	SER	H	143	-8.357	64.979	74.460	1.00	48.43	C
ATOM	6645	C	SER	H	143	-7.504	65.399	75.643	1.00	48.58	C
ATOM	6646	O	SER	H	143	-7.116	64.559	76.459	1.00	48.13	O
ATOM	6647	CB	SER	H	143	-9.846	65.061	74.821	1.00	49.31	C
ATOM	6648	OG	SER	H	143	-10.651	65.255	73.666	1.00	50.90	O
ATOM	6649	N	LYS	H	144	-7.167	66.683	75.709	1.00	49.12	N
ATOM	6650	CA	LYS	H	144	-6.349	67.202	76.800	1.00	49.89	C
ATOM	6651	C	LYS	H	144	-6.844	66.662	78.140	1.00	51.31	C
ATOM	6652	O	LYS	H	144	-6.090	66.025	78.869	1.00	51.30	O
ATOM	6653	CB	LYS	H	144	-6.360	68.734	76.790	1.00	49.53	C
ATOM	6654	CG	LYS	H	144	-5.683	69.354	75.575	1.00	48.06	C
ATOM	6655	CD	LYS	H	144	-4.186	69.080	75.567	1.00	46.41	C
ATOM	6656	CE	LYS	H	144	-3.546	69.638	74.306	1.00	45.68	C
ATOM	6657	NZ	LYS	H	144	-2.062	69.598	74.338	1.00	43.77	N
ATOM	6658	N	SER	H	145	-8.114	66.901	78.452	1.00	52.64	N
ATOM	6659	CA	SER	H	145	-8.684	66.399	79.694	1.00	53.40	C
ATOM	6660	C	SER	H	145	-9.201	64.985	79.410	1.00	52.91	C
ATOM	6661	O	SER	H	145	-9.725	64.713	78.321	1.00	52.97	O
ATOM	6662	CB	SER	H	145	-9.821	67.306	80.178	1.00	53.39	C
ATOM	6663	OG	SER	H	145	-9.400	68.652	80.327	1.00	54.54	O
ATOM	6664	N	THR	H	146	-9.018	64.086	80.371	1.00	51.26	N
ATOM	6665	CA	THR	H	146	-9.450	62.701	80.234	1.00	49.59	C
ATOM	6666	C	THR	H	146	-9.988	62.200	81.572	1.00	49.59	C
ATOM	6667	O	THR	H	146	-10.211	62.993	82.493	1.00	49.78	O
ATOM	6668	CB	THR	H	146	-8.270	61.814	79.808	1.00	48.67	C
ATOM	6669	OG1	THR	H	146	-7.096	62.216	80.523	1.00	47.79	O
ATOM	6670	CG2	THR	H	146	-8.021	61.923	78.309	1.00	48.73	C
ATOM	6671	N	SER	H	147	-10.226	60.893	81.675	1.00	48.75	N
ATOM	6672	CA	SER	H	147	-10.729	60.307	82.915	1.00	48.48	C
ATOM	6673	C	SER	H	147	-9.705	60.452	84.038	1.00	48.25	C
ATOM	6674	O	SER	H	147	-8.741	59.683	84.120	1.00	48.10	O
ATOM	6675	CB	SER	H	147	-11.084	58.830	82.714	1.00	48.05	C
ATOM	6676	OG	SER	H	147	-12.328	58.685	82.040	1.00	48.59	O
ATOM	6677	N	GLY	H	148	-9.905	61.464	84.878	1.00	47.37	N
ATOM	6678	CA	GLY	H	148	-9.002	61.708	85.989	1.00	45.76	C
ATOM	6679	C	GLY	H	148	-8.209	62.980	85.779	1.00	44.78	C
ATOM	6680	O	GLY	H	148	-8.181	63.845	86.644	1.00	44.91	O
ATOM	6681	N	GLY	H	149	-7.554	63.086	84.629	1.00	43.88	N
ATOM	6682	CA	GLY	H	149	-6.772	64.273	84.333	1.00	42.23	C
ATOM	6683	C	GLY	H	149	-5.403	63.928	83.793	1.00	40.65	C
ATOM	6684	O	GLY	H	149	-4.541	64.800	83.623	1.00	40.43	O
ATOM	6685	N	THR	H	150	-5.210	62.642	83.537	1.00	39.02	N
ATOM	6686	CA	THR	H	150	-3.963	62.119	83.016	1.00	36.37	C
ATOM	6687	C	THR	H	150	-4.241	61.693	81.581	1.00	34.47	C
ATOM	6688	O	THR	H	150	-5.009	60.757	81.337	1.00	34.73	O
ATOM	6689	CB	THR	H	150	-3.477	60.881	83.842	1.00	36.14	C
ATOM	6690	OG1	THR	H	150	-3.512	61.180	85.248	1.00	32.44	O
ATOM	6691	CG2	THR	H	150	-2.051	60.496	83.455	1.00	35.60	C
ATOM	6692	N	ALA	H	151	-3.677	62.424	80.630	1.00	32.10	N
ATOM	6693	CA	ALA	H	151	-3.851	62.098	79.227	1.00	30.67	C
ATOM	6694	C	ALA	H	151	-3.236	60.725	78.973	1.00	30.16	C
ATOM	6695	O	ALA	H	151	-2.532	60.176	79.827	1.00	29.46	O
ATOM	6696	CB	ALA	H	151	-3.168	63.150	78.352	1.00	29.03	C
ATOM	6697	N	ALA	H	152	-3.531	60.163	77.810	1.00	29.66	N
ATOM	6698	CA	ALA	H	152	-2.993	58.870	77.422	1.00	28.48	C
ATOM	6699	C	ALA	H	152	-2.818	58.876	75.914	1.00	27.26	C
ATOM	6700	O	ALA	H	152	-3.712	59.305	75.181	1.00	27.16	O
ATOM	6701	CB	ALA	H	152	-3.935	57.748	77.844	1.00	29.31	C
ATOM	6702	N	LEU	H	153	-1.636	58.480	75.466	1.00	26.25	N
ATOM	6703	CA	LEU	H	153	-1.332	58.415	74.043	1.00	25.79	C
ATOM	6704	C	LEU	H	153	-0.510	57.154	73.767	1.00	24.66	C
ATOM	6705	O	LEU	H	153	-0.178	56.417	74.696	1.00	24.12	O
ATOM	6706	CB	LEU	H	153	-0.605	59.693	73.567	1.00	26.39	C
ATOM	6707	CG	LEU	H	153	0.650	60.312	74.186	1.00	25.96	C

FIG. 53-103

ATOM	6709	CD2	LEU	H	153	1.847	59.368	74.110	1.00	28.30	C
ATOM	6710	N	GLY	H	154	-0.213	56.880	72.502	1.00	23.70	N
ATOM	6711	CA	GLY	H	154	0.568	55.697	72.199	1.00	22.99	C
ATOM	6712	C	GLY	H	154	0.875	55.459	70.737	1.00	22.92	C
ATOM	6713	O	GLY	H	154	0.891	56.396	69.927	1.00	21.74	O
ATOM	6714	N	CYS	H	155	1.088	54.190	70.398	1.00	22.73	N
ATOM	6715	CA	CYS	H	155	1.406	53.791	69.035	1.00	21.51	C
ATOM	6716	C	CYS	H	155	0.773	52.453	68.655	1.00	20.37	C
ATOM	6717	O	CYS	H	155	0.755	51.514	69.458	1.00	21.44	O
ATOM	6718	CB	CYS	H	155	2.928	53.684	68.853	1.00	22.18	C
ATOM	6719	SG	CYS	H	155	3.784	55.277	68.636	1.00	25.02	S
ATOM	6720	N	LEU	H	156	0.194	52.407	67.459	1.00	17.40	N
ATOM	6721	CA	LEU	H	156	-0.396	51.203	66.903	1.00	14.77	C
ATOM	6722	C	LEU	H	156	0.707	50.685	65.992	1.00	13.15	C
ATOM	6723	O	LEU	H	156	1.110	51.366	65.050	1.00	11.25	O
ATOM	6724	CB	LEU	H	156	-1.646	51.530	66.065	1.00	14.58	C
ATOM	6725	CG	LEU	H	156	-2.451	50.371	65.437	1.00	13.68	C
ATOM	6726	CD1	LEU	H	156	-3.148	49.517	66.505	1.00	12.41	C
ATOM	6727	CD2	LEU	H	156	-3.485	50.923	64.475	1.00	10.42	C
ATOM	6728	N	VAL	H	157	1.267	49.533	66.343	1.00	13.00	N
ATOM	6729	CA	VAL	H	157	2.329	48.913	65.561	1.00	10.97	C
ATOM	6730	C	VAL	H	157	1.674	47.722	64.892	1.00	10.83	C
ATOM	6731	O	VAL	H	157	1.675	46.626	65.449	1.00	13.03	O
ATOM	6732	CB	VAL	H	157	3.463	48.425	66.469	1.00	10.06	C
ATOM	6733	CG1	VAL	H	157	4.626	47.971	65.649	1.00	9.37	C
ATOM	6734	CG2	VAL	H	157	3.887	49.530	67.421	1.00	12.85	C
ATOM	6735	N	LYS	H	158	1.100	47.943	63.710	1.00	9.96	N
ATOM	6736	CA	LYS	H	158	0.398	46.889	62.993	1.00	8.89	C
ATOM	6737	C	LYS	H	158	0.992	46.427	61.655	1.00	9.25	C
ATOM	6738	O	LYS	H	158	1.905	47.043	61.107	1.00	9.17	O
ATOM	6739	CB	LYS	H	158	-1.081	47.277	62.828	1.00	7.35	C
ATOM	6740	CG	LYS	H	158	-1.459	47.925	61.516	1.00	4.06	C
ATOM	6741	CD	LYS	H	158	-2.926	48.374	61.537	1.00	2.31	C
ATOM	6742	CE	LYS	H	158	-3.910	47.219	61.613	1.00	2.00	C
ATOM	6743	NZ	LYS	H	158	-4.065	46.520	60.303	1.00	4.12	N
ATOM	6744	N	ASP	H	159	0.487	45.288	61.186	1.00	10.34	N
ATOM	6745	CA	ASP	H	159	0.883	44.650	59.938	1.00	9.94	C
ATOM	6746	C	ASP	H	159	2.340	44.239	59.779	1.00	10.44	C
ATOM	6747	O	ASP	H	159	2.940	44.406	58.708	1.00	10.80	O
ATOM	6748	CB	ASP	H	159	0.383	45.448	58.733	1.00	9.84	C
ATOM	6749	CG	ASP	H	159	-1.138	45.491	58.658	1.00	12.75	C
ATOM	6750	OD1	ASP	H	159	-1.806	44.831	59.489	1.00	11.14	O
ATOM	6751	OD2	ASP	H	159	-1.687	46.194	57.782	1.00	14.15	O
ATOM	6752	N	TYR	H	160	2.906	43.680	60.845	1.00	11.17	N
ATOM	6753	CA	TYR	H	160	4.285	43.184	60.809	1.00	12.41	C
ATOM	6754	C	TYR	H	160	4.167	41.673	60.919	1.00	11.93	C
ATOM	6755	O	TYR	H	160	3.183	41.164	61.464	1.00	10.90	O
ATOM	6756	CB	TYR	H	160	5.160	43.768	61.933	1.00	12.71	C
ATOM	6757	CG	TYR	H	160	4.765	43.387	63.337	1.00	13.00	C
ATOM	6758	CD1	TYR	H	160	3.718	44.035	63.984	1.00	13.98	C
ATOM	6759	CD2	TYR	H	160	5.451	42.385	64.029	1.00	12.39	C
ATOM	6760	CE1	TYR	H	160	3.362	43.698	65.291	1.00	13.65	C
ATOM	6761	CE2	TYR	H	160	5.106	42.047	65.326	1.00	11.41	C
ATOM	6762	CZ	TYR	H	160	4.062	42.705	65.956	1.00	11.70	C
ATOM	6763	OH	TYR	H	160	3.719	42.379	67.250	1.00	12.51	O
ATOM	6764	N	PHE	H	161	5.137	40.948	60.374	1.00	13.91	N
ATOM	6765	CA	PHE	H	161	5.042	39.501	60.418	1.00	15.66	C
ATOM	6766	C	PHE	H	161	5.775	38.788	61.543	1.00	17.16	C
ATOM	6767	O	PHE	H	161	5.145	38.450	62.549	1.00	19.68	O
ATOM	6768	CB	PHE	H	161	5.302	38.854	59.044	1.00	14.33	C
ATOM	6769	CG	PHE	H	161	5.267	37.354	59.073	1.00	12.76	C
ATOM	6770	CD1	PHE	H	161	4.191	36.688	59.644	1.00	12.11	C
ATOM	6771	CD2	PHE	H	161	6.352	36.607	58.619	1.00	12.73	C
ATOM	6772	CE1	PHE	H	161	4.201	35.301	59.764	1.00	11.53	C
ATOM	6773	CE2	PHE	H	161	6.369	35.220	58.735	1.00	10.89	C
ATOM	6774	CZ	PHE	H	161	5.297	34.567	59.313	1.00	10.41	C
ATOM	6775	N	PRO	H	162	7.096	38.532	61.412	1.00	16.48	N
ATOM	6776	CA	PRO	H	162	7.687	37.832	62.559	1.00	15.52	C
ATOM	6777	C	PRO	H	162	7.440	38.626	63.839	1.00	16.26	C
ATOM	6778	O	PRO	H	162	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	O

FIG. 53-104

ATOM	6780	CG	PRO	H	162	9.121	37.678	60.688	1.00	15.53	C
ATOM	6781	CD	PRO	H	162	8.115	38.768	60.375	1.00	15.70	C
ATOM	6782	N	GLN	H	163	6.838	37.953	64.821	1.00	17.27	N
ATOM	6783	CA	GLN	H	163	6.465	38.532	66.112	1.00	18.22	C
ATOM	6784	C	GLN	H	163	7.433	39.454	66.869	1.00	18.88	C
ATOM	6785	O	GLN	H	163	7.040	40.541	67.326	1.00	19.04	O
ATOM	6786	CB	GLN	H	163	5.993	37.428	67.058	1.00	18.98	C
ATOM	6787	CG	GLN	H	163	4.617	37.668	67.637	1.00	18.94	C
ATOM	6788	CD	GLN	H	163	4.561	38.878	68.535	1.00	19.62	C
ATOM	6789	OE1	GLN	H	163	4.408	38.753	69.752	1.00	21.57	O
ATOM	6790	NE2	GLN	H	163	4.667	40.062	67.947	1.00	17.24	N
ATOM	6791	N	PRO	H	164	8.697	39.036	67.022	1.00	17.42	N
ATOM	6792	CA	PRO	H	164	9.683	39.851	67.741	1.00	16.50	C
ATOM	6793	C	PRO	H	164	9.767	41.348	67.396	1.00	16.72	C
ATOM	6794	O	PRO	H	164	10.544	41.766	66.526	1.00	15.30	O
ATOM	6795	CB	PRO	H	164	10.992	39.117	67.465	1.00	17.30	C
ATOM	6796	CG	PRO	H	164	10.703	38.336	66.175	1.00	17.74	C
ATOM	6797	CD	PRO	H	164	9.327	37.847	66.419	1.00	15.64	C
ATOM	6798	N	VAL	H	165	8.979	42.147	68.120	1.00	17.00	N
ATOM	6799	CA	VAL	H	165	8.946	43.604	67.968	1.00	14.97	C
ATOM	6800	C	VAL	H	165	9.136	44.216	69.370	1.00	14.98	C
ATOM	6801	O	VAL	H	165	8.626	43.680	70.360	1.00	15.43	O
ATOM	6802	CB	VAL	H	165	7.600	44.100	67.334	1.00	12.34	C
ATOM	6803	CG1	VAL	H	165	6.629	44.578	68.403	1.00	10.73	C
ATOM	6804	CG2	VAL	H	165	7.861	45.207	66.331	1.00	10.36	C
ATOM	6805	N	THR	H	166	9.928	45.283	69.458	1.00	14.94	N
ATOM	6806	CA	THR	H	166	10.173	45.969	70.732	1.00	14.09	C
ATOM	6807	C	THR	H	166	9.767	47.421	70.588	1.00	13.15	C
ATOM	6808	O	THR	H	166	10.005	48.033	69.547	1.00	13.03	O
ATOM	6809	CB	THR	H	166	11.651	45.926	71.164	1.00	14.47	C
ATOM	6810	OG1	THR	H	166	12.466	46.558	70.169	1.00	15.67	O
ATOM	6811	CG2	THR	H	166	12.107	44.490	71.373	1.00	13.84	C
ATOM	6812	N	VAL	H	167	9.151	47.967	71.631	1.00	12.92	N
ATOM	6813	CA	VAL	H	167	8.701	49.352	71.608	1.00	12.11	C
ATOM	6814	C	VAL	H	167	9.166	50.088	72.854	1.00	10.91	C
ATOM	6815	O	VAL	H	167	9.146	49.536	73.948	1.00	11.06	O
ATOM	6816	CB	VAL	H	167	7.159	49.444	71.498	1.00	13.51	C
ATOM	6817	CG1	VAL	H	167	6.716	50.908	71.454	1.00	13.75	C
ATOM	6818	CG2	VAL	H	167	6.669	48.691	70.257	1.00	11.11	C
ATOM	6819	N	SER	H	168	9.617	51.323	72.673	1.00	12.04	N
ATOM	6820	CA	SER	H	168	10.087	52.156	73.779	1.00	12.70	C
ATOM	6821	C	SER	H	168	9.495	53.551	73.632	1.00	11.89	C
ATOM	6822	O	SER	H	168	8.862	53.873	72.622	1.00	10.00	O
ATOM	6823	CB	SER	H	168	11.624	52.277	73.764	1.00	13.07	C
ATOM	6824	OG	SER	H	168	12.261	51.022	73.603	1.00	16.68	O
ATOM	6825	N	TRP	H	169	9.771	54.388	74.625	1.00	13.49	N
ATOM	6826	CA	TRP	H	169	9.307	55.769	74.659	1.00	14.33	C
ATOM	6827	C	TRP	H	169	10.484	56.641	75.061	1.00	13.65	C
ATOM	6828	O	TRP	H	169	11.248	56.284	75.972	1.00	13.91	O
ATOM	6829	CB	TRP	H	169	8.173	55.929	75.669	1.00	16.34	C
ATOM	6830	CG	TRP	H	169	6.913	55.288	75.213	1.00	19.47	C
ATOM	6831	CD1	TRP	H	169	6.441	54.060	75.562	1.00	19.30	C
ATOM	6832	CD2	TRP	H	169	5.985	55.820	74.259	1.00	21.40	C
ATOM	6833	NE1	TRP	H	169	5.284	53.784	74.877	1.00	22.35	N
ATOM	6834	CE2	TRP	H	169	4.979	54.850	74.070	1.00	22.25	C
ATOM	6835	CE3	TRP	H	169	5.910	57.022	73.539	1.00	23.11	C
ATOM	6836	CZ2	TRP	H	169	3.907	55.045	73.191	1.00	22.21	C
ATOM	6837	CZ3	TRP	H	169	4.846	57.214	72.667	1.00	22.11	C
ATOM	6838	CH2	TRP	H	169	3.861	56.229	72.501	1.00	21.83	C
ATOM	6839	N	ASN	H	170	10.630	57.773	74.373	1.00	11.73	N
ATOM	6840	CA	ASN	H	170	11.706	58.722	74.628	1.00	10.55	C
ATOM	6841	C	ASN	H	170	13.056	58.024	74.701	1.00	10.89	C
ATOM	6842	O	ASN	H	170	13.839	58.260	75.630	1.00	9.68	O
ATOM	6843	CB	ASN	H	170	11.472	59.481	75.932	1.00	11.66	C
ATOM	6844	CG	ASN	H	170	10.272	60.394	75.885	1.00	12.60	C
ATOM	6845	OD1	ASN	H	170	9.860	60.911	76.914	1.00	14.09	O
ATOM	6846	ND2	ASN	H	170	9.725	60.626	74.706	1.00	13.33	N
ATOM	6847	N	SER	H	171	13.294	57.113	73.763	1.00	11.69	N
ATOM	6848	CA	SER	H	171	14.547	56.376	73.704	1.00	12.66	C
ATOM	6849	C	SER	H	171	14.977	55.805	75.070	1.00	11.53	C

FIG. 53-105

ATOM	6851	CB	SER	H	171	15.617	57.293	73.128	1.00	13.68	C
ATOM	6852	OG	SER	H	171	15.110	57.967	71.982	1.00	14.88	O
ATOM	6853	N	GLY	H	172	13.999	55.278	75.811	1.00	11.14	N
ATOM	6854	CA	GLY	H	172	14.253	54.675	77.112	1.00	9.53	C
ATOM	6855	C	GLY	H	172	14.197	55.608	78.307	1.00	9.53	C
ATOM	6856	O	GLY	H	172	14.357	55.167	79.452	1.00	8.14	O
ATOM	6857	N	ALA	H	173	13.970	56.892	78.049	1.00	9.47	N
ATOM	6858	CA	ALA	H	173	13.912	57.909	79.109	1.00	10.56	C
ATOM	6859	C	ALA	H	173	12.587	57.852	79.857	1.00	10.20	C
ATOM	6860	O	ALA	H	173	12.496	58.160	81.055	1.00	8.98	O
ATOM	6861	CB	ALA	H	173	14.121	59.297	78.512	1.00	9.38	C
ATOM	6862	N	LEU	H	174	11.551	57.500	79.110	1.00	10.48	N
ATOM	6863	CA	LEU	H	174	10.214	57.369	79.642	1.00	10.25	C
ATOM	6864	C	LEU	H	174	9.955	55.868	79.744	1.00	11.08	C
ATOM	6865	O	LEU	H	174	10.124	55.132	78.768	1.00	11.25	O
ATOM	6866	CB	LEU	H	174	9.216	58.042	78.699	1.00	6.90	C
ATOM	6867	CG	LEU	H	174	7.736	57.832	78.977	1.00	5.18	C
ATOM	6868	CD1	LEU	H	174	7.406	58.185	80.411	1.00	6.39	C
ATOM	6869	CD2	LEU	H	174	6.917	58.650	78.007	1.00	4.39	C
ATOM	6870	N	THR	H	175	9.630	55.416	80.950	1.00	13.76	N
ATOM	6871	CA	THR	H	175	9.348	54.005	81.208	1.00	15.62	C
ATOM	6872	C	THR	H	175	8.210	53.801	82.219	1.00	17.32	C
ATOM	6873	O	THR	H	175	7.619	52.718	82.289	1.00	19.37	O
ATOM	6874	CB	THR	H	175	10.615	53.264	81.703	1.00	13.60	C
ATOM	6875	OG1	THR	H	175	11.353	54.117	82.587	1.00	13.52	O
ATOM	6876	CG2	THR	H	175	11.502	52.870	80.532	1.00	9.95	C
ATOM	6877	N	SER	H	176	7.888	54.831	82.994	1.00	17.59	N
ATOM	6878	CA	SER	H	176	6.811	54.700	83.973	1.00	17.83	C
ATOM	6879	C	SER	H	176	5.425	54.960	83.361	1.00	16.06	C
ATOM	6880	O	SER	H	176	5.265	55.846	82.528	1.00	13.90	O
ATOM	6881	CB	SER	H	176	7.058	55.604	85.190	1.00	18.75	C
ATOM	6882	OG	SER	H	176	7.703	56.822	84.833	1.00	23.79	O
ATOM	6883	N	GLY	H	177	4.451	54.129	83.733	1.00	15.54	N
ATOM	6884	CA	GLY	H	177	3.096	54.271	83.225	1.00	15.16	C
ATOM	6885	C	GLY	H	177	2.816	53.621	81.878	1.00	15.96	C
ATOM	6886	O	GLY	H	177	1.648	53.469	81.494	1.00	14.91	O
ATOM	6887	N	VAL	H	178	3.872	53.198	81.177	1.00	16.41	N
ATOM	6888	CA	VAL	H	178	3.737	52.579	79.854	1.00	16.11	C
ATOM	6889	C	VAL	H	178	3.096	51.190	79.873	1.00	15.06	C
ATOM	6890	O	VAL	H	178	3.199	50.452	80.853	1.00	16.45	O
ATOM	6891	CB	VAL	H	178	5.103	52.495	79.106	1.00	16.24	C
ATOM	6892	CG1	VAL	H	178	5.816	53.841	79.137	1.00	14.61	C
ATOM	6893	CG2	VAL	H	178	5.979	51.406	79.707	1.00	17.09	C
ATOM	6894	N	HIS	H	179	2.451	50.842	78.769	1.00	13.81	N
ATOM	6895	CA	HIS	H	179	1.770	49.563	78.612	1.00	12.20	C
ATOM	6896	C	HIS	H	179	1.917	49.074	77.179	1.00	11.92	C
ATOM	6897	O	HIS	H	179	1.301	49.630	76.279	1.00	10.81	O
ATOM	6898	CB	HIS	H	179	0.268	49.723	78.865	1.00	10.78	C
ATOM	6899	CG	HIS	H	179	-0.089	50.040	80.288	1.00	8.98	C
ATOM	6900	ND1	HIS	H	179	0.744	49.786	81.344	1.00	8.13	N
ATOM	6901	CD2	HIS	H	179	-1.230	50.550	80.810	1.00	7.69	C
ATOM	6902	CE1	HIS	H	179	0.135	50.122	82.475	1.00	7.19	C
ATOM	6903	NE2	HIS	H	179	-1.057	50.586	82.174	1.00	6.91	N
ATOM	6904	N	THR	H	180	2.722	48.044	76.955	1.00	12.23	N
ATOM	6905	CA	THR	H	180	2.866	47.510	75.609	1.00	13.23	C
ATOM	6906	C	THR	H	180	2.130	46.173	75.592	1.00	12.61	C
ATOM	6907	O	THR	H	180	2.649	45.154	76.040	1.00	13.86	O
ATOM	6908	CB	THR	H	180	4.343	47.363	75.216	1.00	13.85	C
ATOM	6909	OG1	THR	H	180	4.978	48.652	75.308	1.00	14.97	O
ATOM	6910	CG2	THR	H	180	4.465	46.841	73.784	1.00	8.77	C
ATOM	6911	N	PHE	H	181	0.887	46.206	75.127	1.00	11.37	N
ATOM	6912	CA	PHE	H	181	0.039	45.025	75.100	1.00	10.00	C
ATOM	6913	C	PHE	H	181	0.611	43.950	74.220	1.00	10.71	C
ATOM	6914	O	PHE	H	181	1.166	44.243	73.168	1.00	11.45	O
ATOM	6915	CB	PHE	H	181	-1.374	45.398	74.630	1.00	8.58	C
ATOM	6916	CG	PHE	H	181	-2.042	46.412	75.503	1.00	6.96	C
ATOM	6917	CD1	PHE	H	181	-2.736	46.017	76.643	1.00	5.39	C
ATOM	6918	CD2	PHE	H	181	-1.904	47.767	75.243	1.00	5.58	C
ATOM	6919	CE1	PHE	H	181	-3.273	46.959	77.514	1.00	2.00	C
ATOM	6920	CE2	PHE	H	181	-2.441	48.708	76.113	1.00	4.38	C

FIG. 53-106

ATOM	6922	N	PRO	H	182	0.505	42.681	74.653	1.00	11.10	N
ATOM	6923	CA	PRO	H	182	1.014	41.533	73.896	1.00	10.01	C
ATOM	6924	C	PRO	H	182	0.447	41.543	72.495	1.00	8.35	C
ATOM	6925	O	PRO	H	182	-0.682	41.975	72.282	1.00	8.98	O
ATOM	6926	CB	PRO	H	182	0.472	40.341	74.688	1.00	10.33	C
ATOM	6927	CG	PRO	H	182	0.481	40.839	76.085	1.00	8.56	C
ATOM	6928	CD	PRO	H	182	-0.093	42.240	75.926	1.00	10.78	C
ATOM	6929	N	ALA	H	183	1.225	41.056	71.543	1.00	7.01	N
ATOM	6930	CA	ALA	H	183	0.789	41.014	70.153	1.00	5.50	C
ATOM	6931	C	ALA	H	183	-0.441	40.154	69.880	1.00	4.29	C
ATOM	6932	O	ALA	H	183	-0.716	39.167	70.571	1.00	5.06	O
ATOM	6933	CB	ALA	H	183	1.924	40.560	69.276	1.00	4.84	C
ATOM	6934	N	VAL	H	184	-1.168	40.539	68.847	1.00	3.67	N
ATOM	6935	CA	VAL	H	184	-2.355	39.827	68.422	1.00	3.96	C
ATOM	6936	C	VAL	H	184	-2.137	39.463	66.960	1.00	5.83	C
ATOM	6937	O	VAL	H	184	-1.449	40.187	66.234	1.00	8.89	O
ATOM	6938	CB	VAL	H	184	-3.580	40.729	68.560	1.00	3.97	C
ATOM	6939	CG1	VAL	H	184	-4.584	40.470	67.447	1.00	6.95	C
ATOM	6940	CG2	VAL	H	184	-4.220	40.506	69.907	1.00	6.37	C
ATOM	6941	N	LEU	H	185	-2.656	38.316	66.536	1.00	6.33	N
ATOM	6942	CA	LEU	H	185	-2.518	37.905	65.141	1.00	4.96	C
ATOM	6943	C	LEU	H	185	-3.812	38.263	64.423	1.00	5.98	C
ATOM	6944	O	LEU	H	185	-4.911	37.958	64.908	1.00	4.69	O
ATOM	6945	CB	LEU	H	185	-2.276	36.401	65.027	1.00	3.01	C
ATOM	6946	CG	LEU	H	185	-1.861	35.914	63.639	1.00	2.00	C
ATOM	6947	CD1	LEU	H	185	-0.558	36.576	63.252	1.00	2.00	C
ATOM	6948	CD2	LEU	H	185	-1.705	34.409	63.639	1.00	2.00	C
ATOM	6949	N	GLN	H	186	-3.685	38.984	63.317	1.00	6.25	N
ATOM	6950	CA	GLN	H	186	-4.846	39.362	62.536	1.00	7.15	C
ATOM	6951	C	GLN	H	186	-5.151	38.230	61.558	1.00	8.80	C
ATOM	6952	O	GLN	H	186	-4.271	37.427	61.232	1.00	9.09	O
ATOM	6953	CB	GLN	H	186	-4.576	40.660	61.782	1.00	4.80	C
ATOM	6954	CG	GLN	H	186	-4.362	41.856	62.690	1.00	4.42	C
ATOM	6955	CD	GLN	H	186	-3.792	43.050	61.959	1.00	2.12	C
ATOM	6956	OE1	GLN	H	186	-4.382	44.142	61.954	1.00	2.81	O
ATOM	6957	NE2	GLN	H	186	-2.618	42.868	61.376	1.00	2.00	N
ATOM	6958	N	SER	H	187	-6.388	38.198	61.064	1.00	9.24	N
ATOM	6959	CA	SER	H	187	-6.829	37.197	60.110	1.00	8.26	C
ATOM	6960	C	SER	H	187	-5.997	37.221	58.828	1.00	7.98	C
ATOM	6961	O	SER	H	187	-6.087	36.311	58.006	1.00	8.54	O
ATOM	6962	CB	SER	H	187	-8.304	37.416	59.794	1.00	10.14	C
ATOM	6963	OG	SER	H	187	-9.040	37.613	60.998	1.00	15.53	O
ATOM	6964	N	SER	H	188	-5.205	38.272	58.648	1.00	7.78	N
ATOM	6965	CA	SER	H	188	-4.338	38.390	57.481	1.00	7.43	C
ATOM	6966	C	SER	H	188	-2.977	37.694	57.665	1.00	6.97	C
ATOM	6967	O	SER	H	188	-2.128	37.727	56.776	1.00	8.42	O
ATOM	6968	CB	SER	H	188	-4.133	39.866	57.143	1.00	8.65	C
ATOM	6969	OG	SER	H	188	-3.836	40.617	58.306	1.00	12.26	O
ATOM	6970	N	GLY	H	189	-2.765	37.073	58.818	1.00	5.75	N
ATOM	6971	CA	GLY	H	189	-1.511	36.395	59.063	1.00	3.96	C
ATOM	6972	C	GLY	H	189	-0.463	37.311	59.648	1.00	5.18	C
ATOM	6973	O	GLY	H	189	0.610	36.862	60.042	1.00	5.52	O
ATOM	6974	N	LEU	H	190	-0.777	38.600	59.711	1.00	6.43	N
ATOM	6975	CA	LEU	H	190	0.132	39.614	60.239	1.00	6.25	C
ATOM	6976	C	LEU	H	190	-0.247	39.977	61.677	1.00	6.30	C
ATOM	6977	O	LEU	H	190	-1.422	39.913	62.037	1.00	6.57	O
ATOM	6978	CB	LEU	H	190	0.023	40.872	59.377	1.00	7.09	C
ATOM	6979	CG	LEU	H	190	0.258	40.789	57.866	1.00	5.45	C
ATOM	6980	CD1	LEU	H	190	-0.363	41.995	57.184	1.00	2.55	C
ATOM	6981	CD2	LEU	H	190	1.745	40.694	57.578	1.00	5.29	C
ATOM	6982	N	TYR	H	191	0.726	40.385	62.489	1.00	8.66	N
ATOM	6983	CA	TYR	H	191	0.444	40.772	63.880	1.00	10.43	C
ATOM	6984	C	TYR	H	191	0.209	42.274	64.038	1.00	11.98	C
ATOM	6985	O	TYR	H	191	0.459	43.062	63.124	1.00	12.48	O
ATOM	6986	CB	TYR	H	191	1.581	40.371	64.820	1.00	10.83	C
ATOM	6987	CG	TYR	H	191	1.822	38.890	64.959	1.00	11.84	C
ATOM	6988	CD1	TYR	H	191	1.091	38.120	65.858	1.00	12.41	C
ATOM	6989	CD2	TYR	H	191	2.820	38.267	64.226	1.00	13.05	C
ATOM	6990	CE1	TYR	H	191	1.362	36.767	66.026	1.00	11.97	C
ATOM	6991	CE2	TYR	H	191	3.096	36.924	64.383	1.00	12.23	C

FIG. 53-107

ATOM	6993	OH	TYR	H	191	2.690	34.852	65.455	1.00	13.42	O
ATOM	6994	N	SER	H	192	-0.202	42.662	65.237	1.00	14.02	N
ATOM	6995	CA	SER	H	192	-0.475	44.052	65.563	1.00	14.64	C
ATOM	6996	C	SER	H	192	-0.597	44.200	67.088	1.00	15.31	C
ATOM	6997	O	SER	H	192	-1.139	43.313	67.758	1.00	15.02	O
ATOM	6998	CB	SER	H	192	-1.785	44.467	64.889	1.00	14.74	C
ATOM	6999	OG	SER	H	192	-2.113	45.824	65.137	1.00	16.74	O
ATOM	7000	N	LEU	H	193	-0.066	45.295	67.632	1.00	15.60	N
ATOM	7001	CA	LEU	H	193	-0.142	45.569	69.075	1.00	15.39	C
ATOM	7002	C	LEU	H	193	-0.047	47.077	69.316	1.00	15.95	C
ATOM	7003	O	LEU	H	193	0.371	47.834	68.425	1.00	14.03	O
ATOM	7004	CB	LEU	H	193	0.984	44.865	69.850	1.00	13.89	C
ATOM	7005	CG	LEU	H	193	2.386	45.477	69.756	1.00	12.32	C
ATOM	7006	CD1	LEU	H	193	3.292	44.932	70.827	1.00	11.49	C
ATOM	7007	CD2	LEU	H	193	2.979	45.215	68.391	1.00	14.57	C
ATOM	7008	N	SER	H	194	-0.415	47.502	70.522	1.00	15.26	N
ATOM	7009	CA	SER	H	194	-0.375	48.911	70.889	1.00	15.50	C
ATOM	7010	C	SER	H	194	0.456	49.149	72.141	1.00	14.88	C
ATOM	7011	O	SER	H	194	0.453	48.343	73.081	1.00	14.55	O
ATOM	7012	CB	SER	H	194	-1.793	49.456	71.118	1.00	15.26	C
ATOM	7013	OG	SER	H	194	-2.572	49.370	69.940	1.00	16.76	O
ATOM	7014	N	SER	H	195	1.180	50.259	72.135	1.00	14.05	N
ATOM	7015	CA	SER	H	195	2.001	50.649	73.261	1.00	14.24	C
ATOM	7016	C	SER	H	195	1.432	52.002	73.664	1.00	14.14	C
ATOM	7017	O	SER	H	195	1.392	52.928	72.850	1.00	15.25	O
ATOM	7018	CB	SER	H	195	3.467	50.773	72.832	1.00	14.96	C
ATOM	7019	OG	SER	H	195	4.326	51.016	73.938	1.00	17.50	O
ATOM	7020	N	VAL	H	196	0.923	52.087	74.888	1.00	13.38	N
ATOM	7021	CA	VAL	H	196	0.327	53.313	75.399	1.00	12.73	C
ATOM	7022	C	VAL	H	196	0.981	53.782	76.689	1.00	13.33	C
ATOM	7023	O	VAL	H	196	1.380	52.975	77.517	1.00	12.87	O
ATOM	7024	CB	VAL	H	196	-1.182	53.146	75.652	1.00	10.44	C
ATOM	7025	CG1	VAL	H	196	-1.889	52.794	74.354	1.00	5.83	C
ATOM	7026	CG2	VAL	H	196	-1.428	52.102	76.735	1.00	8.37	C
ATOM	7027	N	VAL	H	197	1.102	55.097	76.834	1.00	14.77	N
ATOM	7028	CA	VAL	H	197	1.700	55.707	78.014	1.00	15.10	C
ATOM	7029	C	VAL	H	197	0.783	56.824	78.482	1.00	15.44	C
ATOM	7030	O	VAL	H	197	0.309	57.632	77.682	1.00	14.98	O
ATOM	7031	CB	VAL	H	197	3.130	56.261	77.725	1.00	15.42	C
ATOM	7032	CG1	VAL	H	197	3.111	57.210	76.547	1.00	15.39	C
ATOM	7033	CG2	VAL	H	197	3.709	56.938	78.965	1.00	15.02	C
ATOM	7034	N	THR	H	198	0.465	56.802	79.768	1.00	16.66	N
ATOM	7035	CA	THR	H	198	-0.398	57.794	80.358	1.00	19.74	C
ATOM	7036	C	THR	H	198	0.461	58.898	80.955	1.00	22.76	C
ATOM	7037	O	THR	H	198	1.408	58.632	81.692	1.00	25.76	O
ATOM	7038	CB	THR	H	198	-1.289	57.161	81.426	1.00	19.71	C
ATOM	7039	OG1	THR	H	198	-0.484	56.422	82.354	1.00	21.22	O
ATOM	7040	CG2	THR	H	198	-2.286	56.214	80.773	1.00	22.04	C
ATOM	7041	N	VAL	H	199	0.150	60.137	80.612	1.00	23.28	N
ATOM	7042	CA	VAL	H	199	0.910	61.271	81.096	1.00	24.42	C
ATOM	7043	C	VAL	H	199	-0.061	62.386	81.446	1.00	27.05	C
ATOM	7044	O	VAL	H	199	-1.167	62.431	80.904	1.00	26.19	O
ATOM	7045	CB	VAL	H	199	1.918	61.766	80.019	1.00	23.66	C
ATOM	7046	CG1	VAL	H	199	3.062	60.785	79.886	1.00	23.42	C
ATOM	7047	CG2	VAL	H	199	1.227	61.944	78.671	1.00	20.39	C
ATOM	7048	N	PRO	H	200	0.305	63.255	82.413	1.00	28.35	N
ATOM	7049	CA	PRO	H	200	-0.574	64.357	82.804	1.00	28.32	C
ATOM	7050	C	PRO	H	200	-0.874	65.244	81.613	1.00	28.33	C
ATOM	7051	O	PRO	H	200	-0.023	65.424	80.738	1.00	27.57	O
ATOM	7052	CB	PRO	H	200	0.249	65.090	83.866	1.00	28.33	C
ATOM	7053	CG	PRO	H	200	1.656	64.759	83.517	1.00	28.29	C
ATOM	7054	CD	PRO	H	200	1.557	63.300	83.187	1.00	29.22	C
ATOM	7055	N	SER	H	201	-2.091	65.776	81.578	1.00	29.98	N
ATOM	7056	CA	SER	H	201	-2.551	66.652	80.500	1.00	31.65	C
ATOM	7057	C	SER	H	201	-1.697	67.918	80.328	1.00	32.66	C
ATOM	7058	O	SER	H	201	-1.690	68.541	79.265	1.00	31.83	O
ATOM	7059	CB	SER	H	201	-4.005	67.052	80.762	1.00	32.43	C
ATOM	7060	OG	SER	H	201	-4.777	65.936	81.176	1.00	32.44	O
ATOM	7061	N	SER	H	202	-0.983	68.283	81.387	1.00	34.02	N
ATOM	7062	CA	SER	H	202	-0.126	69.460	81.401	1.00	35.50	C

FIG. 53-108

ATOM	7064	O	SER	H	202	1.696	70.292	80.088	1.00	36.22	O
ATOM	7065	CB	SER	H	202	0.165	69.844	82.850	1.00	36.50	C
ATOM	7066	OG	SER	H	202	0.318	68.681	83.651	1.00	38.01	O
ATOM	7067	N	SER	H	203	1.737	68.105	80.597	1.00	36.04	N
ATOM	7068	CA	SER	H	203	2.997	67.854	79.898	1.00	35.59	C
ATOM	7069	C	SER	H	203	2.866	68.019	78.389	1.00	35.77	C
ATOM	7070	O	SER	H	203	3.743	68.590	77.731	1.00	37.10	O
ATOM	7071	CB	SER	H	203	3.511	66.449	80.216	1.00	34.75	C
ATOM	7072	OG	SER	H	203	3.809	66.309	81.597	1.00	36.94	O
ATOM	7073	N	LEU	H	204	1.763	67.518	77.846	1.00	34.93	N
ATOM	7074	CA	LEU	H	204	1.498	67.584	76.418	1.00	34.76	C
ATOM	7075	C	LEU	H	204	1.857	68.962	75.865	1.00	35.53	C
ATOM	7076	O	LEU	H	204	1.592	69.990	76.496	1.00	36.23	O
ATOM	7077	CB	LEU	H	204	0.023	67.282	76.156	1.00	33.94	C
ATOM	7078	CG	LEU	H	204	-0.537	66.058	76.892	1.00	34.12	C
ATOM	7079	CD1	LEU	H	204	-2.018	65.881	76.600	1.00	32.48	C
ATOM	7080	CD2	LEU	H	204	0.243	64.821	76.493	1.00	34.75	C
ATOM	7081	N	GLY	H	205	2.465	68.985	74.688	1.00	35.90	N
ATOM	7082	CA	GLY	H	205	2.856	70.251	74.099	1.00	36.54	C
ATOM	7083	C	GLY	H	205	4.241	70.646	74.581	1.00	36.78	C
ATOM	7084	O	GLY	H	205	5.156	70.809	73.771	1.00	37.69	O
ATOM	7085	N	THR	H	206	4.404	70.790	75.894	1.00	35.10	N
ATOM	7086	CA	THR	H	206	5.698	71.148	76.461	1.00	32.96	C
ATOM	7087	C	THR	H	206	6.646	69.985	76.180	1.00	31.40	C
ATOM	7088	O	THR	H	206	7.620	70.121	75.430	1.00	31.35	O
ATOM	7089	CB	THR	H	206	5.609	71.339	77.981	1.00	32.63	C
ATOM	7090	OG1	THR	H	206	4.294	71.778	78.339	1.00	33.03	O
ATOM	7091	CG2	THR	H	206	6.613	72.379	78.433	1.00	34.20	C
ATOM	7092	N	GLN	H	207	6.352	68.847	76.802	1.00	29.76	N
ATOM	7093	CA	GLN	H	207	7.125	67.625	76.633	1.00	27.98	C
ATOM	7094	C	GLN	H	207	6.445	66.797	75.552	1.00	28.19	C
ATOM	7095	O	GLN	H	207	5.266	66.456	75.674	1.00	28.33	O
ATOM	7096	CB	GLN	H	207	7.161	66.839	77.946	1.00	26.33	C
ATOM	7097	CG	GLN	H	207	7.669	65.415	77.825	1.00	26.06	C
ATOM	7098	CD	GLN	H	207	9.110	65.326	77.354	1.00	25.96	C
ATOM	7099	OE1	GLN	H	207	9.438	65.706	76.225	1.00	25.74	O
ATOM	7100	NE2	GLN	H	207	9.981	64.821	78.220	1.00	24.52	N
ATOM	7101	N	THR	H	208	7.167	66.542	74.467	1.00	28.37	N
ATOM	7102	CA	THR	H	208	6.642	65.752	73.355	1.00	27.66	C
ATOM	7103	C	THR	H	208	6.928	64.277	73.646	1.00	27.73	C
ATOM	7104	O	THR	H	208	7.574	63.952	74.647	1.00	29.05	O
ATOM	7105	CB	THR	H	208	7.276	66.182	72.006	1.00	27.09	C
ATOM	7106	OG1	THR	H	208	8.658	65.799	71.961	1.00	26.14	O
ATOM	7107	CG2	THR	H	208	7.184	67.696	71.834	1.00	25.02	C
ATOM	7108	N	TYR	H	209	6.455	63.381	72.791	1.00	26.40	N
ATOM	7109	CA	TYR	H	209	6.666	61.956	73.026	1.00	25.94	C
ATOM	7110	C	TYR	H	209	6.940	61.150	71.770	1.00	25.67	C
ATOM	7111	O	TYR	H	209	6.332	61.382	70.725	1.00	23.61	O
ATOM	7112	CB	TYR	H	209	5.477	61.366	73.785	1.00	24.52	C
ATOM	7113	CG	TYR	H	209	5.357	61.911	75.181	1.00	25.18	C
ATOM	7114	CD1	TYR	H	209	6.143	61.402	76.210	1.00	25.69	C
ATOM	7115	CD2	TYR	H	209	4.492	62.967	75.468	1.00	24.68	C
ATOM	7116	CE1	TYR	H	209	6.080	61.926	77.493	1.00	27.59	C
ATOM	7117	CE2	TYR	H	209	4.418	63.502	76.750	1.00	27.78	C
ATOM	7118	CZ	TYR	H	209	5.216	62.977	77.760	1.00	28.92	C
ATOM	7119	OH	TYR	H	209	5.168	63.507	79.034	1.00	30.88	O
ATOM	7120	N	ILE	H	210	7.844	60.183	71.892	1.00	26.57	N
ATOM	7121	CA	ILE	H	210	8.219	59.342	70.764	1.00	28.79	C
ATOM	7122	C	ILE	H	210	8.228	57.863	71.134	1.00	28.99	C
ATOM	7123	O	ILE	H	210	8.675	57.492	72.224	1.00	28.57	O
ATOM	7124	CB	ILE	H	210	9.631	59.697	70.253	1.00	29.02	C
ATOM	7125	CG1	ILE	H	210	9.696	61.169	69.845	1.00	29.17	C
ATOM	7126	CG2	ILE	H	210	10.011	58.787	69.084	1.00	28.88	C
ATOM	7127	CD1	ILE	H	210	11.100	61.672	69.602	1.00	28.35	C
ATOM	7128	N	CYS	H	211	7.705	57.030	70.236	1.00	29.45	N
ATOM	7129	CA	CYS	H	211	7.703	55.584	70.449	1.00	29.08	C
ATOM	7130	C	CYS	H	211	8.668	54.952	69.438	1.00	28.27	C
ATOM	7131	O	CYS	H	211	8.516	55.106	68.223	1.00	27.49	O
ATOM	7132	CB	CYS	H	211	6.301	54.986	70.296	1.00	27.46	C
ATOM	7133	SG	CYS	H	211	5.745	54.792	68.581	1.00	26.97	S

FIG. 53-109

ATOM	7135	CA	ASN	H	212	10.712	53.667	69.120	1.00	25.61	C
ATOM	7136	C	ASN	H	212	10.248	52.238	68.890	1.00	23.30	C
ATOM	7137	O	ASN	H	212	10.024	51.495	69.844	1.00	22.85	O
ATOM	7138	CB	ASN	H	212	12.062	53.698	69.828	1.00	27.19	C
ATOM	7139	CG	ASN	H	212	12.313	55.016	70.536	1.00	28.04	C
ATOM	7140	OD1	ASN	H	212	12.541	55.051	71.752	1.00	28.39	O
ATOM	7141	ND2	ASN	H	212	12.235	56.112	69.792	1.00	27.04	N
ATOM	7142	N	VAL	H	213	10.053	51.881	67.627	1.00	21.53	N
ATOM	7143	CA	VAL	H	213	9.582	50.553	67.248	1.00	20.85	C
ATOM	7144	C	VAL	H	213	10.627	49.769	66.460	1.00	19.23	C
ATOM	7145	O	VAL	H	213	10.848	50.030	65.281	1.00	18.38	O
ATOM	7146	CB	VAL	H	213	8.303	50.662	66.411	1.00	21.35	C
ATOM	7147	CG1	VAL	H	213	7.799	49.279	66.026	1.00	21.26	C
ATOM	7148	CG2	VAL	H	213	7.249	51.447	67.181	1.00	20.95	C
ATOM	7149	N	ASN	H	214	11.277	48.817	67.114	1.00	19.12	N
ATOM	7150	CA	ASN	H	214	12.304	48.021	66.447	1.00	19.03	C
ATOM	7151	C	ASN	H	214	11.766	46.667	66.013	1.00	17.33	C
ATOM	7152	O	ASN	H	214	10.867	46.098	66.638	1.00	14.41	O
ATOM	7153	CB	ASN	H	214	13.527	47.837	67.353	1.00	21.24	C
ATOM	7154	CG	ASN	H	214	14.671	47.096	66.665	1.00	22.32	C
ATOM	7155	OD1	ASN	H	214	15.508	47.701	65.997	1.00	22.05	O
ATOM	7156	ND2	ASN	H	214	14.733	45.787	66.863	1.00	23.88	N
ATOM	7157	N	HIS	H	215	12.340	46.157	64.934	1.00	17.25	N
ATOM	7158	CA	HIS	H	215	11.954	44.879	64.381	1.00	16.34	C
ATOM	7159	C	HIS	H	215	13.189	44.329	63.672	1.00	17.87	C
ATOM	7160	O	HIS	H	215	13.558	44.796	62.597	1.00	18.68	O
ATOM	7161	CB	HIS	H	215	10.814	45.071	63.386	1.00	13.92	C
ATOM	7162	CG	HIS	H	215	10.074	43.812	63.062	1.00	12.54	C
ATOM	7163	ND1	HIS	H	215	9.309	43.668	61.930	1.00	14.48	N
ATOM	7164	CD2	HIS	H	215	9.968	42.642	63.740	1.00	12.09	C
ATOM	7165	CE1	HIS	H	215	8.755	42.471	61.919	1.00	12.28	C
ATOM	7166	NE2	HIS	H	215	9.140	41.828	63.010	1.00	11.26	N
ATOM	7167	N	LYS	H	216	13.852	43.367	64.300	1.00	19.14	N
ATOM	7168	CA	LYS	H	216	15.038	42.761	63.726	1.00	21.68	C
ATOM	7169	C	LYS	H	216	14.739	41.988	62.435	1.00	22.97	C
ATOM	7170	O	LYS	H	216	15.407	42.187	61.417	1.00	22.37	O
ATOM	7171	CB	LYS	H	216	15.691	41.834	64.750	1.00	24.90	C
ATOM	7172	CG	LYS	H	216	17.172	41.612	64.539	1.00	30.77	C
ATOM	7173	CD	LYS	H	216	17.978	42.274	65.654	1.00	36.75	C
ATOM	7174	CE	LYS	H	216	17.728	43.785	65.754	1.00	40.46	C
ATOM	7175	NZ	LYS	H	216	18.392	44.376	66.961	1.00	41.89	N
ATOM	7176	N	PRO	H	217	13.699	41.128	62.440	1.00	23.59	N
ATOM	7177	CA	PRO	H	217	13.375	40.358	61.234	1.00	23.65	C
ATOM	7178	C	PRO	H	217	13.316	41.168	59.944	1.00	24.82	C
ATOM	7179	O	PRO	H	217	13.583	40.637	58.861	1.00	26.99	O
ATOM	7180	CB	PRO	H	217	12.021	39.754	61.578	1.00	22.68	C
ATOM	7181	CG	PRO	H	217	12.155	39.488	63.032	1.00	22.06	C
ATOM	7182	CD	PRO	H	217	12.763	40.781	63.527	1.00	23.22	C
ATOM	7183	N	SER	H	218	12.974	42.448	60.050	1.00	24.15	N
ATOM	7184	CA	SER	H	218	12.874	43.288	58.861	1.00	23.21	C
ATOM	7185	C	SER	H	218	13.905	44.412	58.831	1.00	25.33	C
ATOM	7186	O	SER	H	218	13.905	45.235	57.904	1.00	25.52	O
ATOM	7187	CB	SER	H	218	11.461	43.862	58.752	1.00	17.61	C
ATOM	7188	OG	SER	H	218	11.070	44.463	59.971	1.00	10.47	O
ATOM	7189	N	ASN	H	219	14.811	44.409	59.812	1.00	26.07	N
ATOM	7190	CA	ASN	H	219	15.826	45.448	59.928	1.00	25.29	C
ATOM	7191	C	ASN	H	219	15.117	46.793	59.950	1.00	23.66	C
ATOM	7192	O	ASN	H	219	15.470	47.714	59.219	1.00	22.34	O
ATOM	7193	CB	ASN	H	219	16.799	45.383	58.755	1.00	28.99	C
ATOM	7194	CG	ASN	H	219	18.008	44.531	59.051	1.00	30.63	C
ATOM	7195	OD1	ASN	H	219	17.883	43.369	59.422	1.00	31.67	O
ATOM	7196	ND2	ASN	H	219	19.193	45.106	58.888	1.00	32.29	N
ATOM	7197	N	THR	H	220	14.084	46.870	60.775	1.00	22.97	N
ATOM	7198	CA	THR	H	220	13.286	48.066	60.907	1.00	23.30	C
ATOM	7199	C	THR	H	220	13.308	48.621	62.322	1.00	24.58	C
ATOM	7200	O	THR	H	220	13.240	47.882	63.312	1.00	23.13	O
ATOM	7201	CB	THR	H	220	11.805	47.805	60.526	1.00	21.35	C
ATOM	7202	OG1	THR	H	220	11.733	47.337	59.180	1.00	21.56	O
ATOM	7203	CG2	THR	H	220	10.976	49.068	60.638	1.00	21.72	C
ATOM	7204	N	LYS	H	221	13.436	49.941	62.381	1.00	26.22	N

FIG. 53-110

ATOM	7206	C	LYS	H	221	12.739	51.993	63.162	1.00	26.45	C
ATOM	7207	O	LYS	H	221	13.098	52.556	62.127	1.00	26.86	O
ATOM	7208	CB	LYS	H	221	14.816	50.988	64.151	1.00	25.28	C
ATOM	7209	CG	LYS	H	221	14.777	51.554	65.556	1.00	26.33	C
ATOM	7210	CD	LYS	H	221	16.133	51.589	66.222	1.00	28.37	C
ATOM	7211	CE	LYS	H	221	16.033	52.340	67.539	1.00	29.82	C
ATOM	7212	NZ	LYS	H	221	17.288	52.295	68.330	1.00	29.18	N
ATOM	7213	N	VAL	H	222	11.692	52.384	63.870	1.00	26.93	N
ATOM	7214	CA	VAL	H	222	10.946	53.579	63.524	1.00	28.68	C
ATOM	7215	C	VAL	H	222	10.596	54.378	64.770	1.00	29.43	C
ATOM	7216	O	VAL	H	222	10.227	53.815	65.798	1.00	29.62	O
ATOM	7217	CB	VAL	H	222	9.624	53.210	62.819	1.00	29.88	C
ATOM	7218	CG1	VAL	H	222	8.837	54.465	62.460	1.00	29.69	C
ATOM	7219	CG2	VAL	H	222	9.896	52.356	61.598	1.00	29.32	C
ATOM	7220	N	ASP	H	223	10.697	55.693	64.670	1.00	31.29	N
ATOM	7221	CA	ASP	H	223	10.362	56.567	65.784	1.00	31.74	C
ATOM	7222	C	ASP	H	223	9.114	57.323	65.316	1.00	31.35	C
ATOM	7223	O	ASP	H	223	8.960	57.595	64.125	1.00	30.17	O
ATOM	7224	CB	ASP	H	223	11.531	57.519	66.073	1.00	32.60	C
ATOM	7225	CG	ASP	H	223	12.876	56.792	66.178	1.00	31.98	C
ATOM	7226	OD1	ASP	H	223	13.230	56.319	67.280	1.00	29.31	O
ATOM	7227	OD2	ASP	H	223	13.580	56.699	65.149	1.00	32.64	O
ATOM	7228	N	LYS	H	224	8.198	57.602	66.234	1.00	31.93	N
ATOM	7229	CA	LYS	H	224	6.964	58.291	65.883	1.00	34.40	C
ATOM	7230	C	LYS	H	224	6.479	59.180	67.021	1.00	36.63	C
ATOM	7231	O	LYS	H	224	6.118	58.690	68.101	1.00	35.77	O
ATOM	7232	CB	LYS	H	224	5.880	57.267	65.535	1.00	35.25	C
ATOM	7233	CG	LYS	H	224	4.519	57.856	65.198	1.00	35.97	C
ATOM	7234	CD	LYS	H	224	4.544	58.580	63.863	1.00	38.19	C
ATOM	7235	CE	LYS	H	224	3.171	59.133	63.515	1.00	39.84	C
ATOM	7236	NZ	LYS	H	224	3.031	59.588	62.104	1.00	39.10	N
ATOM	7237	N	LYS	H	225	6.497	60.489	66.781	1.00	38.47	N
ATOM	7238	CA	LYS	H	225	6.047	61.450	67.777	1.00	40.00	C
ATOM	7239	C	LYS	H	225	4.532	61.513	67.761	1.00	40.56	C
ATOM	7240	O	LYS	H	225	3.919	61.593	66.690	1.00	40.71	O
ATOM	7241	CB	LYS	H	225	6.627	62.842	67.512	1.00	41.38	C
ATOM	7242	CG	LYS	H	225	6.069	63.928	68.438	1.00	43.12	C
ATOM	7243	CD	LYS	H	225	6.731	65.280	68.225	1.00	44.83	C
ATOM	7244	CE	LYS	H	225	8.227	65.214	68.501	1.00	46.17	C
ATOM	7245	NZ	LYS	H	225	8.872	66.552	68.416	1.00	47.79	N
ATOM	7246	N	VAL	H	226	3.937	61.450	68.946	1.00	41.43	N
ATOM	7247	CA	VAL	H	226	2.490	61.514	69.071	1.00	42.84	C
ATOM	7248	C	VAL	H	226	2.073	62.974	69.216	1.00	44.17	C
ATOM	7249	O	VAL	H	226	2.381	63.628	70.218	1.00	43.46	O
ATOM	7250	CB	VAL	H	226	1.979	60.701	70.279	1.00	41.78	C
ATOM	7251	CG1	VAL	H	226	0.472	60.507	70.172	1.00	40.41	C
ATOM	7252	CG2	VAL	H	226	2.687	59.358	70.353	1.00	40.96	C
ATOM	7253	N	GLU	H	227	1.435	63.494	68.176	1.00	45.83	N
ATOM	7254	CA	GLU	H	227	0.971	64.873	68.156	1.00	46.70	C
ATOM	7255	C	GLU	H	227	-0.179	65.042	69.132	1.00	47.48	C
ATOM	7256	O	GLU	H	227	-1.005	64.151	69.290	1.00	48.42	O
ATOM	7257	CB	GLU	H	227	0.557	65.306	66.733	1.00	46.15	C
ATOM	7258	CG	GLU	H	227	-0.282	64.301	65.931	1.00	45.39	C
ATOM	7259	CD	GLU	H	227	0.547	63.185	65.312	1.00	44.09	C
ATOM	7260	OE1	GLU	H	227	1.155	63.402	64.243	1.00	44.02	O
ATOM	7261	OE2	GLU	H	227	0.584	62.084	65.894	1.00	42.58	O
ATOM	7262	N	PRO	H	228	-0.237	66.186	69.817	1.00	48.64	N
ATOM	7263	CA	PRO	H	228	-1.297	66.463	70.790	1.00	49.52	C
ATOM	7264	C	PRO	H	228	-2.695	66.664	70.210	1.00	49.89	C
ATOM	7265	O	PRO	H	228	-2.855	67.026	69.044	1.00	48.97	O
ATOM	7266	CB	PRO	H	228	-0.793	67.721	71.482	1.00	50.46	C
ATOM	7267	CG	PRO	H	228	-0.054	68.421	70.378	1.00	50.48	C
ATOM	7268	CD	PRO	H	228	0.722	67.300	69.750	1.00	49.24	C
ATOM	7269	N	LYS	H	229	-3.696	66.420	71.055	1.00	51.01	N
ATOM	7270	CA	LYS	H	229	-5.109	66.571	70.708	1.00	50.89	C
ATOM	7271	C	LYS	H	229	-5.964	66.499	71.975	1.00	49.93	C
ATOM	7272	O	LYS	H	229	-6.378	67.582	72.444	1.00	49.29	O
ATOM	7273	CB	LYS	H	229	-5.560	65.494	69.710	1.00	50.99	C
ATOM	7274	CG	LYS	H	229	-7.049	65.559	69.333	1.00	51.00	C
ATOM	7275	CD	LYS	H	229	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	C

FIG. 53-111

ATOM	7277	NZ	LYS	H	229	-8.352	68.958	70.228	1.00	54.11	N
TER	7278		LYS	H	229						
HETATM	7279	O	HOH		1	22.165	9.529	79.160	1.00	2.00	O
HETATM	7280	O	HOH		2	11.911	1.801	70.392	1.00	6.27	O
HETATM	7281	O	HOH		3	1.103	23.950	73.530	1.00	2.00	O
HETATM	7282	O	HOH		4	13.339	9.604	88.234	1.00	2.00	O
HETATM	7283	O	HOH		5	32.518	-17.948	103.755	1.00	4.10	O
HETATM	7284	O	HOH		6	-25.644	45.440	74.531	1.00	2.00	O
HETATM	7285	O	HOH		7	50.290	18.960	56.862	1.00	2.00	O
HETATM	7286	O	HOH		8	38.873	-2.572	84.241	1.00	2.00	O
HETATM	7287	O	HOH		9	22.766	-42.838	87.811	1.00	4.05	O
HETATM	7288	O	HOH		10	27.297	-7.705	74.948	1.00	2.00	O
HETATM	7289	O	HOH		11	-2.591	36.529	85.413	1.00	2.00	O
HETATM	7290	O	HOH		12	-10.145	19.754	92.343	1.00	2.00	O
HETATM	7291	O	HOH		13	14.134	-5.783	94.278	1.00	2.00	O
HETATM	7292	O	HOH		14	16.122	23.074	97.779	1.00	2.00	O
HETATM	7293	O	HOH		15	17.049	-42.606	77.879	1.00	2.05	O
HETATM	7294	O	HOH		16	37.979	-6.682	96.642	1.00	2.00	O
HETATM	7295	O	HOH		17	-2.446	25.504	77.697	1.00	2.00	O
HETATM	7296	O	HOH		18	19.949	4.273	89.649	1.00	2.13	O
HETATM	7297	O	HOH		19	15.645	5.014	68.450	1.00	2.00	O
HETATM	7298	O	HOH		20	-19.962	42.751	63.628	1.00	2.92	O
HETATM	7299	O	HOH		21	59.945	-15.290	74.664	1.00	2.14	O
HETATM	7300	O	HOH		22	10.277	61.569	79.315	1.00	2.97	O
HETATM	7301	O	HOH		23	-9.504	39.045	92.132	1.00	4.39	O
HETATM	7302	O	HOH		24	-1.295	32.363	59.813	1.00	6.79	O
HETATM	7303	O	HOH		25	-10.346	15.142	92.580	1.00	5.85	O
HETATM	7304	O	HOH		26	43.551	-12.354	97.257	1.00	2.00	O
HETATM	7305	O	HOH		27	59.784	28.541	67.004	1.00	8.19	O
HETATM	7306	O	HOH		28	7.111	18.959	100.259	1.00	3.59	O
HETATM	7307	O	HOH		29	14.885	-24.670	80.511	1.00	8.88	O
HETATM	7308	O	HOH		30	-2.619	64.345	85.123	1.00	2.00	O
HETATM	7309	O	HOH		31	37.275	-15.380	109.070	1.00	2.00	O
HETATM	7310	O	HOH		32	23.327	-9.758	81.087	1.00	5.64	O
HETATM	7311	O	HOH		33	41.146	-13.975	83.133	1.00	8.88	O
HETATM	7312	O	HOH		34	-5.559	35.837	106.706	1.00	2.00	O
HETATM	7313	O	HOH		35	39.858	-31.312	80.857	1.00	2.62	O
HETATM	7314	O	HOH		36	-6.964	34.744	99.440	1.00	6.18	O
HETATM	7315	O	HOH		37	8.406	56.401	59.861	1.00	14.11	O
HETATM	7316	O	HOH		38	28.098	-17.419	68.859	1.00	9.36	O
HETATM	7317	O	HOH		39	7.309	32.808	56.517	1.00	3.40	O
HETATM	7318	O	HOH		40	48.182	18.003	55.687	1.00	5.31	O
HETATM	7319	O	HOH		41	13.560	8.574	76.389	1.00	3.44	O
HETATM	7320	O	HOH		42	44.794	-32.062	86.982	1.00	2.00	O
HETATM	7321	O	HOH		43	3.416	46.935	81.161	1.00	3.06	O
HETATM	7322	O	HOH		44	9.905	58.282	61.578	1.00	6.16	O
HETATM	7323	O	HOH		45	3.954	66.270	66.601	1.00	2.00	O
HETATM	7324	O	HOH		46	34.782	-30.843	80.859	1.00	2.00	O
HETATM	7325	O	HOH		47	6.378	71.557	81.908	1.00	5.92	O
HETATM	7326	O	HOH		48	-10.103	62.639	59.099	1.00	6.28	O
HETATM	7327	O	HOH		49	57.029	-8.449	52.647	1.00	9.33	O
HETATM	7328	O	HOH		50	12.704	-24.369	84.770	1.00	6.18	O
HETATM	7329	O	HOH		51	17.676	15.222	63.164	1.00	3.84	O
HETATM	7330	O	HOH		52	54.823	-7.050	50.766	1.00	2.00	O
HETATM	7331	O	HOH		53	42.016	-32.002	82.471	1.00	2.00	O
HETATM	7332	O	HOH		54	-1.192	9.535	72.350	1.00	7.59	O
HETATM	7333	O	HOH		55	60.614	10.882	65.751	1.00	4.69	O
HETATM	7334	O	HOH		56	4.080	59.007	82.151	1.00	4.10	O
HETATM	7335	O	HOH		57	46.087	-28.223	99.118	1.00	4.68	O
HETATM	7336	O	HOH		58	0.678	37.773	54.674	1.00	2.55	O
HETATM	7337	O	HOH		59	11.861	-0.136	83.796	1.00	2.56	O
HETATM	7338	O	HOH		60	-0.333	44.117	95.564	1.00	10.62	O
HETATM	7339	O	HOH		61	27.052	-12.944	69.452	1.00	7.64	O
HETATM	7340	O	HOH		62	-2.539	47.008	94.502	1.00	12.92	O
HETATM	7341	O	HOH		63	36.964	-23.164	76.315	1.00	4.23	O
HETATM	7342	O	HOH		64	49.693	-12.767	79.396	1.00	8.13	O
HETATM	7343	O	HOH		65	15.462	15.223	80.328	1.00	10.92	O
HETATM	7344	O	HOH		66	62.573	-4.720	59.499	1.00	10.84	O
HETATM	7345	O	HOH		67	5.569	58.370	89.372	1.00	9.52	O
HETATM	7346	O	HOH		68	7.450	43.460	65.953	1.00	9.42	O

FIG. 53-112

HETATM	7348	O	HOH	70	7.955	0.339	72.229	1.00	8.67	O
HETATM	7349	O	HOH	71	14.698	51.000	59.877	1.00	7.66	O
HETATM	7350	O	HOH	72	60.442	14.789	68.692	1.00	13.94	O
HETATM	7351	O	HOH	73	29.550	5.626	76.429	1.00	9.44	O
HETATM	7352	O	HOH	74	23.488	-12.795	103.491	1.00	7.66	O
HETATM	7353	O	HOH	75	55.350	-17.876	76.419	1.00	11.30	O
HETATM	7354	O	HOH	76	-3.980	55.107	64.298	1.00	7.49	O
HETATM	7355	O	HOH	77	31.336	-37.543	88.786	1.00	12.45	O
HETATM	7356	O	HOH	78	53.764	13.270	60.229	1.00	7.00	O
HETATM	7357	O	HOH	79	22.510	-14.728	88.570	1.00	13.52	O
HETATM	7358	O	HOH	80	26.954	18.767	65.939	1.00	10.42	O
HETATM	7359	O	HOH	81	17.435	-24.103	93.619	1.00	11.09	O
HETATM	7360	O	HOH	82	2.324	16.962	77.639	1.00	11.45	O
HETATM	7361	O	HOH	83	42.819	-10.854	76.734	1.00	12.42	O
HETATM	7362	O	HOH	84	19.836	-2.530	99.533	1.00	12.41	O
HETATM	7363	O	HOH	85	17.370	-13.308	101.942	1.00	8.42	O
HETATM	7364	O	HOH	86	11.146	66.878	74.135	1.00	12.89	O
HETATM	7365	O	HOH	87	39.173	-24.013	77.444	1.00	7.92	O
HETATM	7366	O	HOH	88	14.477	24.016	86.336	1.00	10.87	O
HETATM	7367	O	HOH	89	68.983	35.023	53.834	1.00	15.42	O
HETATM	7368	O	HOH	90	66.303	-5.484	68.312	1.00	8.44	O
HETATM	7369	O	HOH	91	69.207	8.623	48.984	1.00	3.58	O
HETATM	7370	O	HOH	92	15.670	1.312	76.211	1.00	7.75	O
HETATM	7371	O	HOH	93	50.357	15.548	50.843	1.00	7.95	O
HETATM	7372	O	HOH	94	-12.212	65.127	77.508	1.00	11.88	O
HETATM	7373	O	HOH	95	10.631	32.727	91.432	1.00	13.61	O
HETATM	7374	O	HOH	96	9.439	9.433	64.343	1.00	13.19	O
HETATM	7375	O	HOH	97	24.875	-30.408	73.942	1.00	6.08	O
HETATM	7376	O	HOH	98	6.838	41.588	69.878	1.00	16.99	O
HETATM	7377	O	HOH	99	13.587	31.324	95.823	1.00	7.70	O
HETATM	7378	O	HOH	100	44.463	-29.489	74.048	1.00	2.00	O
HETATM	7379	O	HOH	101	51.342	1.341	76.032	1.00	10.66	O
HETATM	7380	O	HOH	102	51.212	-28.609	69.751	1.00	16.76	O
HETATM	7381	O	HOH	103	5.423	47.471	55.773	1.00	9.10	O
HETATM	7382	O	HOH	104	-3.178	38.328	73.176	1.00	15.56	O
HETATM	7383	O	HOH	105	10.637	53.193	76.911	1.00	12.15	O
HETATM	7384	O	HOH	106	22.795	-12.364	86.133	1.00	18.01	O
HETATM	7385	O	HOH	107	27.091	-22.792	106.177	1.00	10.59	O
HETATM	7386	O	HOH	108	15.923	23.867	90.058	1.00	13.78	O
HETATM	7387	O	HOH	109	-9.008	13.858	77.706	1.00	8.30	O
HETATM	7388	O	HOH	110	3.704	57.214	61.407	1.00	11.60	O
HETATM	7389	O	HOH	111	-3.669	43.253	55.419	1.00	16.77	O
HETATM	7390	O	HOH	112	33.501	-1.832	86.297	1.00	11.89	O
HETATM	7391	O	HOH	113	42.661	-26.173	71.459	1.00	20.46	O
HETATM	7392	O	HOH	114	31.043	17.252	64.838	1.00	15.53	O
HETATM	7393	O	HOH	115	-4.504	34.542	84.856	1.00	9.88	O
HETATM	7394	O	HOH	116	53.047	23.643	46.970	1.00	10.95	O
HETATM	7395	O	HOH	117	16.022	-19.990	86.523	1.00	15.78	O
HETATM	7396	O	HOH	118	20.590	28.045	81.230	1.00	9.39	O
HETATM	7397	O	HOH	119	48.277	-6.022	83.992	1.00	10.97	O
HETATM	7398	O	HOH	120	57.036	-24.902	98.133	1.00	16.18	O
HETATM	7399	O	HOH	121	5.591	52.123	58.678	1.00	12.13	O
HETATM	7400	O	HOH	122	0.961	35.324	86.508	1.00	15.96	O
HETATM	7401	O	HOH	123	35.507	-25.465	74.447	1.00	16.04	O
HETATM	7402	O	HOH	124	28.949	-14.394	76.841	1.00	11.40	O
HETATM	7403	O	HOH	125	-6.401	60.822	84.877	1.00	17.22	O
HETATM	7404	O	HOH	126	-0.337	46.472	83.468	1.00	11.84	O
HETATM	7405	O	HOH	127	-6.936	34.868	82.669	1.00	21.10	O
HETATM	7406	O	HOH	128	70.351	32.466	57.167	1.00	16.84	O
HETATM	7407	O	HOH	129	42.235	-28.673	72.078	1.00	12.31	O
HETATM	7408	O	HOH	130	27.003	7.858	71.274	1.00	17.91	O
HETATM	7409	O	HOH	131	-20.266	54.933	52.694	1.00	9.75	O
HETATM	7410	O	HOH	132	-4.357	8.994	96.842	1.00	7.58	O
HETATM	7411	O	HOH	133	28.406	-16.947	76.829	1.00	13.90	O
HETATM	7412	O	HOH	134	8.543	58.475	83.123	1.00	10.11	O
HETATM	7413	O	HOH	135	18.494	12.809	61.570	1.00	15.24	O
HETATM	7414	O	HOH	136	28.075	-30.594	95.656	1.00	4.74	O
HETATM	7415	O	HOH	137	42.938	-45.127	78.791	1.00	17.56	O
HETATM	7416	O	HOH	138	28.751	-11.594	107.122	1.00	12.51	O
HETATM	7417	O	HOH	139	42.264	13.006	79.405	1.00	10.56	O

FIG. 53-113

HETATM	7419	O	HOH	141	55.796	-20.368	75.764	1.00	10.04	O
HETATM	7420	O	HOH	142	7.955	3.518	72.301	1.00	15.50	O
HETATM	7421	O	HOH	143	5.388	7.280	69.370	1.00	13.93	O
HETATM	7422	O	HOH	144	50.714	-0.970	55.913	1.00	12.13	O
HETATM	7423	O	HOH	145	11.373	31.813	77.043	1.00	18.74	O
HETATM	7424	O	HOH	146	10.609	65.109	80.839	1.00	15.07	O
HETATM	7425	O	HOH	147	-22.776	48.048	84.973	1.00	13.08	O
HETATM	7426	O	HOH	148	2.152	14.209	63.515	1.00	19.36	O
HETATM	7427	O	HOH	149	28.677	-15.259	109.865	1.00	11.03	O
HETATM	7428	O	HOH	150	55.391	19.247	46.436	1.00	11.06	O
HETATM	7429	O	HOH	151	54.946	-11.772	89.245	1.00	22.22	O
HETATM	7430	O	HOH	152	27.897	19.384	78.558	1.00	18.71	O
HETATM	7431	O	HOH	153	-23.058	54.253	79.253	1.00	14.83	O
HETATM	7432	O	HOH	154	29.804	25.684	81.988	1.00	17.86	O
HETATM	7433	O	HOH	155	33.062	-0.846	92.984	1.00	8.46	O
HETATM	7434	O	HOH	156	-10.657	11.384	84.281	1.00	12.49	O
HETATM	7435	O	HOH	157	12.381	27.954	90.699	1.00	17.73	O
HETATM	7436	O	HOH	158	13.676	44.432	68.890	1.00	11.16	O
HETATM	7437	O	HOH	159	61.317	37.504	51.767	1.00	13.49	O
HETATM	7438	O	HOH	160	17.791	18.137	95.261	1.00	14.35	O
HETATM	7439	O	HOH	161	14.379	52.980	71.925	1.00	16.56	O
HETATM	7440	O	HOH	162	41.192	-22.679	59.991	1.00	17.07	O
HETATM	7441	O	HOH	163	48.359	-29.507	77.036	1.00	24.31	O
HETATM	7442	O	HOH	164	43.551	-33.235	89.036	1.00	15.63	O
HETATM	7443	O	HOH	165	-19.552	65.707	65.325	1.00	16.30	O
HETATM	7444	O	HOH	166	51.766	-18.992	77.503	1.00	10.87	O
HETATM	7445	O	HOH	167	-7.552	31.531	83.394	1.00	12.41	O
HETATM	7446	O	HOH	168	70.680	23.618	50.621	1.00	10.11	O
HETATM	7447	O	HOH	169	2.712	17.305	94.600	1.00	14.68	O
HETATM	7448	O	HOH	170	24.298	-9.578	68.345	1.00	12.50	O
HETATM	7449	O	HOH	171	0.246	5.938	74.609	1.00	14.87	O
HETATM	7450	O	HOH	172	-5.220	44.555	69.546	1.00	13.80	O
HETATM	7451	O	HOH	173	39.118	-24.386	61.724	1.00	8.70	O
HETATM	7452	O	HOH	174	24.181	-9.027	64.624	1.00	13.71	O
HETATM	7453	O	HOH	175	3.695	39.485	54.069	1.00	15.15	O
HETATM	7454	O	HOH	176	17.117	52.940	61.036	1.00	13.69	O
HETATM	7455	O	HOH	177	10.828	8.090	62.402	1.00	26.25	O
HETATM	7456	O	HOH	178	32.268	-38.218	86.345	1.00	17.93	O
HETATM	7457	O	HOH	179	73.798	27.825	52.191	1.00	24.74	O
HETATM	7458	O	HOH	180	59.358	-4.565	64.787	1.00	15.43	O
HETATM	7459	O	HOH	181	41.535	-2.375	86.744	1.00	7.10	O
HETATM	7460	O	HOH	182	-8.946	29.518	82.336	1.00	15.69	O
HETATM	7461	O	HOH	183	55.326	15.266	47.219	1.00	17.04	O
HETATM	7462	O	HOH	184	29.904	-21.145	109.019	1.00	27.75	O
HETATM	7463	O	HOH	185	2.643	2.395	80.292	1.00	12.45	O
HETATM	7464	O	HOH	186	22.721	-1.471	50.919	1.00	20.96	O
HETATM	7465	O	HOH	187	31.190	15.323	75.128	1.00	20.03	O
HETATM	7466	O	HOH	188	14.972	-3.491	93.351	1.00	14.63	O
HETATM	7467	O	HOH	189	33.643	-26.102	88.928	1.00	13.28	O
HETATM	7468	O	HOH	190	14.157	-3.832	83.653	1.00	15.51	O
HETATM	7469	O	HOH	191	16.075	2.677	84.119	1.00	13.77	O
HETATM	7470	O	HOH	192	5.961	59.756	86.639	1.00	15.45	O
HETATM	7471	O	HOH	193	53.593	7.432	73.872	1.00	9.46	O
HETATM	7472	O	HOH	194	16.552	28.787	80.605	1.00	20.58	O
HETATM	7473	O	HOH	195	-22.154	61.730	66.879	1.00	19.00	O
HETATM	7474	O	HOH	196	65.211	23.556	50.589	1.00	12.65	O
HETATM	7475	O	HOH	197	20.812	-10.237	80.086	1.00	15.99	O
HETATM	7476	O	HOH	198	12.680	-22.809	92.537	1.00	20.01	O
HETATM	7477	O	HOH	199	4.860	39.319	100.878	1.00	17.08	O
HETATM	7478	O	HOH	200	14.643	-8.475	94.915	1.00	16.72	O
HETATM	7479	O	HOH	201	37.171	-16.695	56.371	1.00	25.94	O
HETATM	7480	O	HOH	202	3.554	22.859	104.659	1.00	23.27	O
HETATM	7481	O	HOH	203	13.921	-6.176	85.398	1.00	17.14	O
HETATM	7482	O	HOH	204	-9.333	36.554	63.643	1.00	13.99	O
HETATM	7483	O	HOH	205	41.956	-38.297	93.320	1.00	14.96	O
HETATM	7484	O	HOH	206	12.202	55.926	84.289	1.00	28.63	O
HETATM	7485	O	HOH	207	32.415	-13.038	57.015	1.00	13.94	O
HETATM	7486	O	HOH	208	23.428	26.174	70.332	1.00	20.13	O
HETATM	7487	O	HOH	209	39.691	-2.493	81.540	1.00	12.68	O
HETATM	7488	O	HOH	210	45.745	-6.123	86.144	1.00	15.47	O

FIG. 53-114

HETATM	7490	O	HOH	212	4.232	41.785	93.744	1.00	11.14	O
HETATM	7491	O	HOH	213	-26.371	48.653	83.800	1.00	22.33	O
HETATM	7492	O	HOH	214	35.669	-23.875	104.159	1.00	17.37	O
HETATM	7493	O	HOH	215	-4.831	41.986	98.947	1.00	15.95	O
HETATM	7494	O	HOH	216	64.565	-18.038	83.429	1.00	17.54	O
HETATM	7495	O	HOH	217	11.574	-6.057	93.845	1.00	13.27	O
HETATM	7496	O	HOH	218	16.307	-18.239	94.494	1.00	19.10	O
HETATM	7497	O	HOH	219	11.937	69.635	73.406	1.00	19.30	O
HETATM	7498	O	HOH	220	26.169	-28.822	96.515	1.00	19.46	O
HETATM	7499	O	HOH	221	67.272	34.853	56.556	1.00	21.78	O
HETATM	7500	O	HOH	222	-18.977	59.720	77.820	1.00	22.92	O
HETATM	7501	O	HOH	223	15.918	20.946	99.582	1.00	16.46	O
HETATM	7502	O	HOH	224	-0.774	60.722	61.425	1.00	13.35	O
HETATM	7503	O	HOH	225	43.500	-21.837	105.724	1.00	24.80	O
HETATM	7504	O	HOH	226	-19.597	48.328	89.458	1.00	11.73	O
HETATM	7505	O	HOH	227	4.976	31.168	72.941	1.00	15.48	O
HETATM	7506	O	HOH	228	20.015	10.958	62.951	1.00	18.60	O
HETATM	7507	O	HOH	229	-1.877	27.929	79.869	1.00	11.60	O
HETATM	7508	O	HOH	230	50.008	-13.926	99.678	1.00	18.48	O
HETATM	7509	O	HOH	231	53.017	-6.427	76.116	1.00	13.73	O
HETATM	7510	O	HOH	232	49.120	19.715	51.618	1.00	14.06	O
HETATM	7511	O	HOH	233	71.110	19.870	50.750	1.00	18.75	O
HETATM	7512	O	HOH	234	40.374	-37.587	74.192	1.00	31.35	O
HETATM	7513	O	HOH	235	42.478	-21.001	69.295	1.00	12.38	O
HETATM	7514	O	HOH	236	7.753	59.653	60.902	1.00	17.67	O
HETATM	7515	O	HOH	237	21.916	-47.992	76.997	1.00	24.89	O
HETATM	7516	O	HOH	238	-18.941	54.736	85.871	1.00	20.65	O
HETATM	7517	O	HOH	239	38.415	-43.269	84.655	1.00	25.51	O
HETATM	7518	O	HOH	240	-18.492	48.187	61.040	1.00	24.74	O
HETATM	7519	O	HOH	241	38.277	-50.092	75.188	1.00	19.53	O
HETATM	7520	O	HOH	242	68.758	16.494	47.667	1.00	18.47	O
HETATM	7521	O	HOH	243	24.340	-32.949	92.430	1.00	22.79	O
HETATM	7522	O	HOH	244	6.446	31.879	48.021	1.00	24.85	O
HETATM	7523	O	HOH	245	28.709	11.531	68.166	1.00	16.31	O
HETATM	7524	O	HOH	246	31.753	-18.347	108.363	1.00	16.37	O
HETATM	7525	O	HOH	247	17.759	-8.734	71.761	1.00	26.28	O
HETATM	7526	O	HOH	248	-25.338	48.165	75.161	1.00	15.71	O
HETATM	7527	O	HOH	249	67.204	3.621	65.113	1.00	20.08	O
HETATM	7528	O	HOH	250	3.091	29.574	81.292	1.00	23.58	O
HETATM	7529	O	HOH	251	29.230	-25.705	89.928	1.00	18.11	O
HETATM	7530	O	HOH	252	20.116	-6.764	65.412	1.00	16.66	O
HETATM	7531	O	HOH	253	29.673	-12.800	109.481	1.00	20.49	O
HETATM	7532	O	HOH	254	25.768	10.314	72.068	1.00	13.03	O
HETATM	7533	O	HOH	255	61.202	29.626	44.098	1.00	21.43	O
HETATM	7534	O	HOH	256	2.263	24.087	69.363	1.00	14.58	O
HETATM	7535	O	HOH	257	-3.037	70.229	83.110	1.00	21.27	O
HETATM	7536	O	HOH	258	72.666	33.964	61.263	1.00	36.04	O
HETATM	7537	O	HOH	259	4.432	16.319	101.738	1.00	16.96	O
HETATM	7538	O	HOH	260	-13.423	48.880	72.973	1.00	24.01	O
HETATM	7539	O	HOH	261	-4.663	58.301	66.514	1.00	15.31	O
HETATM	7540	O	HOH	262	40.987	-35.386	93.294	1.00	22.01	O
HETATM	7541	O	HOH	263	-11.233	62.808	76.653	1.00	24.18	O
HETATM	7542	O	HOH	264	24.821	0.548	61.582	1.00	21.73	O
HETATM	7543	O	HOH	265	24.965	29.544	79.722	1.00	22.80	O
HETATM	7544	O	HOH	266	-5.380	3.025	75.813	1.00	22.22	O
HETATM	7545	O	HOH	267	24.742	-24.647	89.587	1.00	20.25	O
HETATM	7546	O	HOH	268	65.140	7.222	49.806	1.00	15.66	O
HETATM	7547	O	HOH	269	41.346	-10.499	81.998	1.00	18.92	O
HETATM	7548	O	HOH	270	66.840	21.038	63.543	1.00	13.26	O
HETATM	7549	O	HOH	271	51.301	-14.931	69.495	1.00	22.63	O
HETATM	7550	O	HOH	272	29.219	-0.500	64.123	1.00	19.73	O
HETATM	7551	O	HOH	273	20.241	6.270	63.246	1.00	13.54	O
HETATM	7552	O	HOH	274	24.373	-49.590	68.733	1.00	17.26	O
HETATM	7553	O	HOH	275	-3.304	48.988	55.440	1.00	31.16	O
HETATM	7554	O	HOH	276	20.108	7.029	66.151	1.00	16.95	O
HETATM	7555	O	HOH	277	7.782	-18.762	93.633	1.00	26.41	O
HETATM	7556	O	HOH	278	27.949	-0.521	45.474	1.00	22.32	O
HETATM	7557	O	HOH	279	31.631	6.490	78.024	1.00	21.67	O
HETATM	7558	O	HOH	280	23.318	29.759	69.062	1.00	22.20	O
HETATM	7559	O	HOH	281	-6.348	20.741	81.137	1.00	24.62	O

FIG. 53-115

HETATM	7561	O	HOH	283	52.122	-23.691	79.136	1.00	23.09	O
HETATM	7562	O	HOH	284	70.779	32.618	51.713	1.00	17.19	O
HETATM	7563	O	HOH	285	63.452	0.172	52.716	1.00	33.32	O
HETATM	7564	O	HOH	286	22.958	-47.681	67.413	1.00	22.89	O
HETATM	7565	O	HOH	287	23.890	32.593	72.960	1.00	22.24	O
HETATM	7566	O	HOH	288	20.986	30.840	66.080	1.00	21.84	O
HETATM	7567	O	HOH	289	-9.603	65.551	84.452	1.00	25.25	O
HETATM	7568	O	HOH	290	28.073	-23.477	89.005	1.00	18.93	O
HETATM	7569	O	HOH	291	55.835	10.701	63.810	1.00	20.35	O
HETATM	7570	O	HOH	292	9.046	17.920	56.027	1.00	15.93	O
HETATM	7571	O	HOH	293	28.350	-18.254	64.363	1.00	15.02	O
HETATM	7572	O	HOH	294	-0.201	3.801	81.142	1.00	16.11	O
HETATM	7573	O	HOH	295	46.141	-21.508	105.098	1.00	16.42	O
HETATM	7574	O	HOH	296	13.399	-22.499	76.433	1.00	25.53	O
HETATM	7575	O	HOH	297	24.981	-30.380	92.166	1.00	33.02	O
HETATM	7576	O	HOH	298	13.771	56.074	62.370	1.00	19.18	O
HETATM	7577	O	HOH	299	-8.893	35.838	86.208	1.00	20.61	O
HETATM	7578	O	HOH	300	-22.126	64.290	67.305	1.00	19.81	O
HETATM	7579	O	HOH	301	33.698	-14.983	108.516	1.00	14.40	O
HETATM	7580	O	HOH	302	42.101	-11.945	58.376	1.00	20.92	O
HETATM	7581	O	HOH	303	-18.526	61.045	73.900	1.00	32.62	O
HETATM	7582	O	HOH	304	3.513	24.995	102.792	1.00	23.31	O
HETATM	7583	O	HOH	305	20.343	18.184	93.670	1.00	17.08	O
HETATM	7584	O	HOH	306	5.882	55.992	87.891	1.00	30.47	O
HETATM	7585	O	HOH	307	-9.244	36.503	67.888	1.00	28.48	O
HETATM	7586	O	HOH	308	-23.036	58.479	59.552	1.00	22.63	O
HETATM	7587	O	HOH	309	-22.227	45.809	59.422	1.00	21.33	O
HETATM	7588	O	HOH	310	53.262	10.903	71.166	1.00	17.46	O
HETATM	7589	O	HOH	311	52.602	26.636	60.251	1.00	25.23	O
HETATM	7590	O	HOH	312	-9.994	55.398	87.998	1.00	17.49	O
HETATM	7591	O	HOH	313	-1.994	61.292	66.107	1.00	21.25	O
HETATM	7592	O	HOH	314	50.016	-11.293	93.731	1.00	24.97	O
HETATM	7593	O	HOH	315	15.116	16.011	100.168	1.00	15.56	O
HETATM	7594	O	HOH	316	-6.826	24.369	98.991	1.00	22.05	O
HETATM	7595	O	HOH	317	2.708	42.709	80.252	1.00	17.54	O
HETATM	7596	O	HOH	318	1.253	20.189	100.045	1.00	15.04	O
HETATM	7597	O	HOH	319	5.356	34.912	77.758	1.00	13.93	O
HETATM	7598	O	HOH	320	28.400	23.106	67.434	1.00	26.44	O
HETATM	7599	O	HOH	321	9.493	-19.687	95.975	1.00	31.85	O
HETATM	7600	O	HOH	322	54.155	24.844	62.487	1.00	16.62	O
HETATM	7601	O	HOH	323	46.411	-19.574	59.883	1.00	31.91	O
HETATM	7602	O	HOH	324	-9.761	37.077	89.314	1.00	28.06	O
HETATM	7603	O	HOH	325	17.686	-11.211	73.805	1.00	18.94	O
HETATM	7604	O	HOH	326	1.967	43.860	93.220	1.00	18.25	O
HETATM	7605	O	HOH	327	6.187	59.026	91.814	1.00	28.67	O
HETATM	7606	O	HOH	328	37.107	-14.358	54.717	1.00	22.03	O
HETATM	7607	O	HOH	329	38.785	-11.357	84.088	1.00	16.84	O
HETATM	7608	O	HOH	330	-16.066	60.369	76.960	1.00	36.78	O
HETATM	7609	O	HOH	331	-5.054	1.253	78.433	1.00	25.45	O
HETATM	7610	O	HOH	332	11.331	-12.981	75.925	1.00	14.82	O
HETATM	7611	O	HOH	333	32.919	-41.920	95.418	1.00	27.83	O
HETATM	7612	O	HOH	334	-14.341	51.888	93.906	1.00	24.92	O
HETATM	7613	O	HOH	335	53.967	-0.127	74.878	1.00	28.14	O
HETATM	7614	O	HOH	336	12.881	-19.058	86.018	1.00	23.40	O
HETATM	7615	O	HOH	337	5.705	51.167	93.636	1.00	19.15	O
HETATM	7616	O	HOH	338	42.319	-33.425	91.495	1.00	24.82	O
HETATM	7617	O	HOH	339	2.306	38.419	86.466	1.00	19.39	O
HETATM	7618	O	HOH	340	43.350	-13.777	74.954	1.00	21.98	O
HETATM	7619	O	HOH	341	33.960	-34.534	91.429	1.00	29.34	O
HETATM	7620	O	HOH	342	4.202	62.085	62.525	1.00	26.90	O
HETATM	7621	O	HOH	343	30.962	-34.415	78.307	1.00	19.88	O
HETATM	7622	O	HOH	344	35.773	-42.848	100.309	1.00	30.39	O
HETATM	7623	O	HOH	345	12.021	-37.942	70.940	1.00	20.13	O
HETATM	7624	O	HOH	346	-1.357	49.449	58.279	1.00	25.11	O
HETATM	7625	O	HOH	347	65.788	2.612	67.270	1.00	26.50	O
HETATM	7626	O	HOH	348	62.163	0.051	71.262	1.00	14.33	O
HETATM	7627	O	HOH	349	3.350	45.790	78.716	1.00	19.58	O
HETATM	7628	O	HOH	350	45.104	-33.566	100.903	1.00	25.20	O
HETATM	7629	O	HOH	351	43.597	-0.623	84.186	1.00	28.63	O
HETATM	7630	O	HOH	352	4.596	12.343	97.087	1.00	25.56	O

FIG. 53-116

HETATM	7632	O	HOH	354	1.875	10.993	64.255	1.00	38.92	O
HETATM	7633	O	HOH	355	14.789	30.075	58.623	1.00	21.49	O
HETATM	7634	O	HOH	356	41.516	-25.204	62.351	1.00	22.09	O
HETATM	7635	O	HOH	357	32.943	-23.386	104.220	1.00	27.01	O
HETATM	7636	O	HOH	358	-10.674	42.191	63.227	1.00	19.76	O
HETATM	7637	O	HOH	359	-13.052	65.840	75.218	1.00	29.44	O
HETATM	7638	O	HOH	360	37.573	-17.256	81.764	1.00	27.76	O
HETATM	7639	O	HOH	361	20.895	9.352	68.130	1.00	16.95	O
HETATM	7640	O	HOH	362	-27.567	46.850	73.499	1.00	27.75	O
HETATM	7641	O	HOH	363	8.363	27.062	51.462	1.00	23.49	O
HETATM	7642	O	HOH	364	20.807	-20.790	92.215	1.00	13.77	O
HETATM	7643	O	HOH	365	38.677	-18.189	74.814	1.00	28.95	O
HETATM	7644	O	HOH	366	-2.447	43.907	70.580	1.00	29.93	O
HETATM	7645	O	HOH	367	64.618	-6.837	66.273	1.00	29.07	O
HETATM	7646	O	HOH	368	-5.882	37.844	71.080	1.00	16.09	O
HETATM	7647	O	HOH	369	11.154	36.109	99.944	1.00	28.58	O
HETATM	7648	O	HOH	370	-5.542	16.069	77.059	1.00	25.73	O
HETATM	7649	O	HOH	371	31.111	-16.478	52.927	1.00	31.54	O
HETATM	7650	O	HOH	372	5.976	50.145	55.972	1.00	20.23	O
HETATM	7651	O	HOH	373	22.475	-11.962	59.589	1.00	25.23	O
HETATM	7652	O	HOH	374	-12.598	60.928	80.629	1.00	31.48	O
HETATM	7653	O	HOH	375	39.980	-5.340	88.804	1.00	25.19	O
HETATM	7654	O	HOH	376	-2.191	22.122	77.573	1.00	19.70	O
HETATM	7655	O	HOH	377	-1.570	23.321	89.728	1.00	27.93	O
HETATM	7656	O	HOH	378	33.278	2.409	86.604	1.00	20.38	O
HETATM	7657	O	HOH	379	39.069	-36.284	69.975	1.00	35.94	O
HETATM	7658	O	HOH	380	37.465	-16.311	88.358	1.00	25.21	O
HETATM	7659	O	HOH	381	-16.777	66.073	65.338	1.00	23.04	O
HETATM	7660	O	HOH	382	64.525	-20.940	83.663	1.00	32.87	O
HETATM	7661	O	HOH	383	20.902	-16.651	86.838	1.00	21.83	O
HETATM	7662	O	HOH	384	17.379	15.560	98.403	1.00	36.64	O
HETATM	7663	O	HOH	385	52.346	-11.927	82.994	1.00	24.35	O
HETATM	7664	O	HOH	386	33.051	-14.312	69.234	1.00	23.31	O
HETATM	7665	O	HOH	387	18.244	-50.461	70.951	1.00	32.07	O
HETATM	7666	O	HOH	388	4.393	13.312	75.485	1.00	27.15	O
HETATM	7667	O	HOH	389	67.585	44.217	58.028	1.00	44.96	O
HETATM	7668	O	HOH	390	4.131	14.065	99.710	1.00	26.76	O
HETATM	7669	O	HOH	391	11.175	-0.969	70.399	1.00	26.13	O
HETATM	7670	O	HOH	392	51.116	-18.029	102.066	1.00	23.76	O
HETATM	7671	O	HOH	393	27.092	-7.580	108.056	1.00	18.96	O
HETATM	7672	O	HOH	394	-0.076	36.263	69.351	1.00	28.76	O
HETATM	7673	O	HOH	395	18.133	0.192	74.686	1.00	26.61	O
HETATM	7674	O	HOH	396	43.049	2.569	79.498	1.00	31.94	O
HETATM	7675	O	HOH	397	-23.286	56.992	79.188	1.00	29.11	O
HETATM	7676	O	HOH	398	-7.488	11.902	76.612	1.00	26.52	O
HETATM	7677	O	HOH	399	-13.380	61.310	72.384	1.00	31.14	O
HETATM	7678	O	HOH	400	27.123	-46.681	87.721	1.00	30.44	O
HETATM	7679	O	HOH	401	29.433	-31.173	89.189	1.00	25.67	O
HETATM	7680	O	HOH	402	52.760	-20.241	79.508	1.00	13.02	O
HETATM	7681	O	HOH	403	-1.394	34.237	85.422	1.00	22.50	O
HETATM	7682	O	HOH	404	23.304	-20.804	99.890	1.00	21.06	O
HETATM	7683	O	HOH	405	10.950	27.172	54.652	1.00	26.13	O
HETATM	7684	O	HOH	406	17.093	-18.459	105.982	1.00	38.33	O
HETATM	7685	O	HOH	407	29.611	-46.659	90.122	1.00	22.95	O
HETATM	7686	O	HOH	408	10.218	70.152	76.785	1.00	48.49	O
HETATM	7687	O	HOH	409	60.036	-4.064	49.508	1.00	35.97	O
HETATM	7688	O	HOH	410	51.542	-26.357	92.153	1.00	37.00	O
HETATM	7689	O	HOH	411	43.954	-25.924	102.957	1.00	25.36	O
HETATM	7690	O	HOH	412	8.761	46.091	74.278	1.00	21.32	O
HETATM	7691	O	HOH	413	25.286	-20.091	69.480	1.00	15.27	O
HETATM	7692	O	HOH	414	65.539	40.531	49.494	1.00	31.85	O
HETATM	7693	O	HOH	415	44.413	-32.734	84.479	1.00	28.75	O
HETATM	7694	O	HOH	416	-5.043	18.491	79.930	1.00	30.44	O
HETATM	7695	O	HOH	417	-3.086	39.625	75.814	1.00	29.90	O
HETATM	7696	O	HOH	418	58.905	-24.381	86.911	1.00	35.04	O
HETATM	7697	O	HOH	419	44.458	-29.330	96.836	1.00	29.99	O
HETATM	7698	O	HOH	420	-19.898	62.569	69.832	1.00	34.66	O
HETATM	7699	O	HOH	421	21.778	-33.633	73.728	1.00	29.63	O
HETATM	7700	O	HOH	422	28.583	-8.540	66.452	1.00	42.51	O
HETATM	7701	O	HOH	423	46.541	8.226	72.813	1.00	42.38	O

FIG. 53-117

HETATM	7703	O	HOH	425	38.290	-25.478	102.465	1.00	30.41	O
HETATM	7704	O	HOH	426	19.472	-12.973	106.738	1.00	26.85	O
HETATM	7705	O	HOH	427	62.854	11.594	46.547	1.00	26.89	O
HETATM	7706	O	HOH	428	31.588	-16.806	71.522	1.00	24.18	O
HETATM	7707	O	HOH	429	13.954	13.665	81.796	1.00	24.37	O
HETATM	7708	O	HOH	430	2.011	5.974	84.071	1.00	28.86	O
HETATM	7709	O	HOH	431	7.560	21.926	104.239	1.00	34.95	O
HETATM	7710	O	HOH	432	14.098	-7.313	91.358	1.00	22.24	O
HETATM	7711	O	HOH	433	32.623	-2.548	91.064	1.00	24.03	O
HETATM	7712	O	HOH	434	4.401	54.311	60.091	1.00	22.83	O
HETATM	7713	O	HOH	435	4.015	35.675	104.766	1.00	19.87	O
HETATM	7714	O	HOH	436	-17.908	53.196	92.502	1.00	38.80	O
HETATM	7715	O	HOH	437	27.675	-50.214	83.317	1.00	28.60	O
HETATM	7716	O	HOH	438	-11.291	59.604	78.311	1.00	16.91	O
HETATM	7717	O	HOH	439	31.453	1.868	91.380	1.00	28.49	O
HETATM	7718	O	HOH	440	-11.594	70.398	81.234	1.00	31.72	O
HETATM	7719	O	HOH	441	46.134	-11.872	61.301	1.00	21.50	O
HETATM	7720	O	HOH	442	11.900	35.238	64.506	1.00	23.66	O
HETATM	7721	O	HOH	443	4.846	10.765	96.924	1.00	34.00	O
HETATM	7722	O	HOH	444	-18.730	59.840	58.173	1.00	43.07	O
HETATM	7723	O	HOH	445	57.404	-16.056	75.983	1.00	42.76	O
HETATM	7724	O	HOH	446	29.809	-16.290	111.959	1.00	48.83	O
HETATM	7725	O	HOH	447	32.033	-44.011	72.701	1.00	24.09	O
HETATM	7726	O	HOH	448	20.875	-24.975	70.063	1.00	48.89	O
HETATM	7727	O	HOH	449	-19.969	46.503	77.606	1.00	25.87	O
HETATM	7728	O	HOH	450	-21.566	54.606	85.472	1.00	40.92	O
HETATM	7729	O	HOH	451	31.102	-32.885	98.369	1.00	11.96	O
HETATM	7730	O	HOH	452	-8.189	9.765	80.662	1.00	35.27	O
HETATM	7731	O	HOH	453	31.340	-19.222	51.487	1.00	24.37	O
HETATM	7732	O	HOH	454	29.058	-28.472	89.087	1.00	26.15	O
HETATM	7733	O	HOH	455	-2.419	36.836	105.573	1.00	27.97	O
HETATM	7734	O	HOH	456	21.812	-9.184	104.095	1.00	27.13	O
HETATM	7735	O	HOH	457	49.451	-20.677	84.809	1.00	41.47	O
HETATM	7736	O	HOH	458	0.747	30.885	63.795	1.00	31.04	O
HETATM	7737	O	HOH	459	-26.174	50.602	73.929	1.00	53.06	O
HETATM	7738	O	HOH	460	8.337	72.878	75.753	1.00	38.38	O
HETATM	7739	O	HOH	461	23.508	-2.410	57.597	1.00	46.06	O
HETATM	7740	O	HOH	462	37.169	-45.172	99.612	1.00	37.17	O
HETATM	7741	O	HOH	463	22.696	-4.544	56.151	1.00	47.00	O
HETATM	7742	O	HOH	464	21.082	-23.510	106.197	1.00	22.09	O
HETATM	7743	O	HOH	465	-3.315	21.210	61.358	1.00	27.90	O
HETATM	7744	O	HOH	466	25.279	-14.132	96.196	1.00	28.85	O
HETATM	7745	O	HOH	467	63.921	40.060	58.906	1.00	35.83	O
HETATM	7746	O	HOH	468	14.094	-6.423	88.307	1.00	44.69	O
HETATM	7747	O	HOH	469	25.519	1.763	92.408	1.00	24.38	O
HETATM	7748	O	HOH	470	50.197	11.830	54.707	1.00	28.25	O
HETATM	7749	O	HOH	471	21.550	31.794	76.291	1.00	21.43	O
HETATM	7750	O	HOH	472	26.886	-15.693	73.749	1.00	41.24	O
HETATM	7751	O	HOH	473	14.177	31.775	80.787	1.00	46.37	O
HETATM	7752	O	HOH	474	-13.585	38.871	87.985	1.00	32.09	O
HETATM	7753	O	HOH	475	41.661	-21.201	71.774	1.00	34.90	O
HETATM	7754	O	HOH	476	48.196	-33.291	70.217	1.00	37.35	O
HETATM	7755	O	HOH	477	0.248	5.883	79.177	1.00	23.06	O
HETATM	7756	O	HOH	478	-20.978	57.784	74.179	1.00	45.09	O
HETATM	7757	O	HOH	479	15.338	14.734	57.576	1.00	27.62	O
HETATM	7758	O	HOH	480	39.859	-43.440	87.980	1.00	30.78	O
HETATM	7759	O	HOH	481	5.332	35.152	64.988	1.00	33.57	O
HETATM	7760	O	HOH	482	32.546	-7.422	108.285	1.00	41.57	O
HETATM	7761	O	HOH	483	20.706	43.978	65.616	1.00	37.68	O
HETATM	7762	O	HOH	484	61.667	39.679	46.403	1.00	37.33	O
HETATM	7763	O	HOH	485	56.153	6.917	74.246	1.00	22.50	O
HETATM	7764	O	HOH	486	7.035	69.370	79.949	1.00	25.17	O
HETATM	7765	O	HOH	487	57.622	33.652	55.881	1.00	33.26	O
HETATM	7766	O	HOH	488	18.571	3.099	54.965	1.00	33.08	O
HETATM	7767	O	HOH	489	0.917	22.142	67.869	1.00	27.76	O
HETATM	7768	O	HOH	490	-10.181	67.927	72.593	1.00	37.33	O
HETATM	7769	O	HOH	491	-1.369	19.165	63.747	1.00	42.82	O
HETATM	7770	O	HOH	492	-2.905	16.592	80.047	1.00	27.79	O
HETATM	7771	O	HOH	493	71.624	17.692	61.442	1.00	30.28	O
HETATM	7772	O	HOH	494	10.989	44.711	55.632	1.00	34.86	O

FIG. 53-118

HETATM	7774	O	HOH	496	56.970	20.418	62.613	1.00	43.51	O
HETATM	7775	O	HOH	497	7.317	61.022	83.606	1.00	30.90	O
HETATM	7776	O	HOH	498	-20.765	57.011	50.630	1.00	30.28	O
HETATM	7777	O	HOH	499	5.680	-5.938	83.013	1.00	33.85	O
HETATM	7778	O	HOH	500	10.160	33.195	64.242	1.00	33.78	O
HETATM	7779	O	HOH	501	-3.876	47.464	68.947	1.00	35.45	O
HETATM	7780	O	HOH	502	25.895	-25.113	107.060	1.00	31.04	O
HETATM	7781	O	HOH	503	25.954	-25.486	96.235	1.00	41.89	O
HETATM	7782	O	HOH	504	11.628	-8.334	83.763	1.00	37.43	O
HETATM	7783	O	HOH	505	20.353	-25.228	99.439	1.00	28.33	O
HETATM	7784	O	HOH	506	74.272	26.082	49.678	1.00	23.93	O
HETATM	7785	O	HOH	507	21.208	-4.593	103.849	1.00	35.84	O
HETATM	7786	O	HOH	508	-11.137	31.147	89.386	1.00	37.60	O
HETATM	7787	O	HOH	509	2.586	5.500	73.452	1.00	22.80	O
HETATM	7788	O	HOH	510	65.236	-3.380	56.556	1.00	40.70	O
HETATM	7789	O	HOH	511	41.003	-32.111	78.380	1.00	43.60	O
HETATM	7790	O	HOH	512	36.216	-35.399	72.031	1.00	27.60	O
HETATM	7791	O	HOH	513	19.195	29.924	79.296	1.00	54.45	O
HETATM	7792	O	HOH	514	33.620	-39.417	97.385	1.00	19.90	O
HETATM	7793	O	HOH	515	42.416	-2.969	83.920	1.00	35.14	O
HETATM	7794	O	HOH	516	17.949	-13.685	90.670	1.00	40.03	O
HETATM	7795	O	HOH	517	3.575	51.449	55.759	1.00	26.16	O
HETATM	7796	O	HOH	518	11.256	2.878	84.105	1.00	23.64	O
HETATM	7797	O	HOH	519	-12.990	55.942	83.392	1.00	29.31	O
HETATM	7798	O	HOH	520	23.910	-7.458	59.473	1.00	49.79	O
HETATM	7799	O	HOH	521	-0.082	9.238	75.111	1.00	30.80	O
HETATM	7800	O	HOH	522	-11.514	65.215	81.280	1.00	40.25	O
HETATM	7801	O	HOH	523	1.302	12.024	74.914	1.00	22.96	O
HETATM	7802	O	HOH	524	-12.681	60.508	63.319	1.00	35.93	O
HETATM	7803	O	HOH	525	26.972	-49.547	86.691	1.00	28.47	O
HETATM	7804	O	HOH	526	27.537	25.048	86.077	1.00	34.16	O
HETATM	7805	O	HOH	527	6.797	56.961	61.831	1.00	42.31	O
HETATM	7806	O	HOH	528	42.484	-2.653	58.047	1.00	40.72	O
HETATM	7807	O	HOH	529	-18.325	52.964	53.615	1.00	39.32	O
HETATM	7808	O	HOH	530	31.179	-21.542	61.949	1.00	33.36	O
HETATM	7809	O	HOH	531	11.810	67.897	76.687	1.00	31.68	O
HETATM	7810	O	HOH	532	7.417	5.985	71.567	1.00	32.02	O
HETATM	7811	O	HOH	533	-21.963	59.779	80.267	1.00	19.20	O
HETATM	7812	O	HOH	534	25.891	3.913	54.668	1.00	39.82	O
HETATM	7813	O	HOH	535	11.470	61.996	73.117	1.00	38.96	O
HETATM	7814	O	HOH	536	32.905	-1.708	70.903	1.00	33.03	O
HETATM	7815	O	HOH	537	44.005	-23.045	60.071	1.00	40.10	O
HETATM	7816	O	HOH	538	-10.255	28.829	87.634	1.00	36.10	O
HETATM	7817	O	HOH	539	16.712	-10.311	97.916	1.00	33.61	O
HETATM	7818	O	HOH	540	41.339	1.249	74.690	1.00	28.48	O
HETATM	7819	O	HOH	541	-1.348	71.272	76.255	1.00	25.11	O
HETATM	7820	O	HOH	542	34.260	17.004	67.448	1.00	38.74	O
HETATM	7821	O	HOH	543	11.605	5.120	70.043	1.00	38.08	O
HETATM	7822	O	HOH	544	52.550	-9.796	53.931	1.00	35.58	O
HETATM	7823	O	HOH	545	14.247	54.880	59.924	1.00	32.50	O
HETATM	7824	O	HOH	546	-2.549	46.429	71.418	1.00	32.37	O
HETATM	7825	O	HOH	547	12.782	-40.884	84.382	1.00	24.04	O
HETATM	7826	O	HOH	548	-25.600	44.661	65.942	1.00	27.28	O
HETATM	7827	O	HOH	549	27.739	-35.104	72.246	1.00	41.35	O
HETATM	7828	O	HOH	550	73.990	31.829	50.606	1.00	36.92	O
HETATM	7829	O	HOH	551	12.894	-10.737	95.923	1.00	36.10	O
HETATM	7830	O	HOH	552	46.236	-9.151	59.517	1.00	38.03	O
HETATM	7831	O	HOH	553	14.123	42.425	67.129	1.00	52.00	O
HETATM	7832	O	HOH	554	-23.813	46.436	79.979	1.00	37.72	O
HETATM	7833	O	HOH	555	-26.297	58.232	78.735	1.00	29.43	O
HETATM	7834	O	HOH	556	35.090	-43.947	90.740	1.00	37.16	O
HETATM	7835	O	HOH	557	66.933	8.617	46.645	1.00	22.50	O
HETATM	7836	O	HOH	558	33.659	-6.348	111.290	1.00	33.71	O
HETATM	7837	O	HOH	559	22.491	-13.967	105.700	1.00	33.38	O
HETATM	7838	O	HOH	560	12.516	-5.293	101.139	1.00	38.89	O
HETATM	7839	O	HOH	561	10.978	32.220	73.143	1.00	39.37	O
HETATM	7840	O	HOH	562	55.531	-10.263	54.745	1.00	41.91	O
HETATM	7841	O	HOH	563	-8.024	12.880	90.645	1.00	33.15	O
HETATM	7842	O	HOH	564	14.873	18.651	98.780	1.00	32.24	O
HETATM	7843	O	HOH	565	41.000	-14.756	57.520	1.00	34.69	O

FIG. 53-119

```
HETATM 7845 O HOH 567 36.171 -1.816 61.767 1.00 31.43 O
HETATM 7846 O HOH 568 44.474 -26.007 60.823 1.00 34.19 O
HETATM 7847 O HOH 569 20.938 -46.385 85.402 1.00 29.47 O
HETATM 7848 O HOH 570 52.948 8.143 71.171 1.00 34.33 O
HETATM 7849 O HOH 571 51.129 -7.179 82.571 1.00 47.80 O
HETATM 7850 O HOH 572 68.198 2.685 52.665 1.00 23.57 O
HETATM 7851 O HOH 573 12.116 71.650 75.451 1.00 46.93 O
HETATM 7852 O HOH 574 62.213 37.792 48.687 1.00 53.82 O
HETATM 7853 O HOH 575 20.495 10.177 90.640 1.00 39.16 O
HETATM 7854 O HOH 576 30.400 -48.938 83.842 1.00 35.90 O
HETATM 7855 O HOH 577 13.579 9.779 62.019 1.00 44.35 O
HETATM 7856 O HOH 578 10.453 26.949 106.358 1.00 40.82 O
HETATM 7857 O HOH 579 60.381 11.598 69.404 1.00 34.68 O
HETATM 7858 O HOH 580 25.629 2.637 73.266 1.00 36.83 O
HETATM 7859 O HOH 581 32.166 -30.120 78.054 1.00 37.93 O
HETATM 7860 O HOH 582 -22.014 44.722 62.268 1.00 30.72 O
HETATM 7861 O HOH 583 11.801 31.240 55.851 1.00 44.26 O
HETATM 7862 O HOH 584 18.441 -32.822 78.003 1.00 44.37 O
HETATM 7863 O HOH 585 30.789 22.569 66.579 1.00 46.89 O
HETATM 7864 O HOH 586 37.285 -23.655 106.529 1.00 30.28 O
HETATM 7865 O HOH 587 51.534 10.981 63.481 1.00 32.89 O
HETATM 7866 O HOH 588 49.912 3.080 78.435 1.00 47.56 O
HETATM 7867 O HOH 589 34.134 -20.660 68.829 1.00 36.65 O
HETATM 7868 O HOH 590 37.754 -14.502 81.017 1.00 37.24 O
HETATM 7869 O HOH 591 36.512 -49.054 82.287 1.00 45.12 O
HETATM 7870 O HOH 592 -5.195 45.154 64.492 1.00 33.46 O
HETATM 7871 O HOH 593 23.758 -22.142 68.735 1.00 46.87 O
HETATM 7872 O HOH 594 11.629 38.685 97.627 1.00 33.19 O
HETATM 7873 O HOH 595 21.263 2.941 69.561 1.00 39.33 O
HETATM 7874 O HOH 596 73.271 25.458 53.024 1.00 25.93 O
HETATM 7875 O HOH 597 45.849 -7.205 101.568 1.00 36.34 O
HETATM 7876 O HOH 598 44.216 -10.630 108.940 1.00 43.94 O
HETATM 7877 O HOH 599 59.076 -22.331 92.759 1.00 47.77 O
HETATM 7878 O HOH 600 54.559 -30.657 83.945 1.00 59.82 O
HETATM 7879 O HOH 601 -1.816 16.701 100.021 1.00 52.67 O
HETATM 7880 O HOH 602 58.154 31.812 65.596 1.00 52.96 O
HETATM 7881 O HOH 1000 26.160 -11.235 84.250 0.00 0.00 O
CONECT 255 254 402
CONECT 307 306 339
CONECT 339 307 338
CONECT 347 345 2302
CONECT 402 255 401
CONECT 509 508 713
CONECT 577 576 656
CONECT 628 626 2316
CONECT 656 577 655
CONECT 713 509 712
CONECT 828 826 2330
CONECT 932 930 2344
CONECT 1035 1033 2358
CONECT 1080 1078 2372
CONECT 1086 1085 1122
CONECT 1122 1086 1121
CONECT 1130 1128 2386
CONECT 1191 1189 2400
CONECT 1496 1495 1926
CONECT 1553 1552 1709
CONECT 1561 1559 2414
CONECT 1610 1608 2428
CONECT 1709 1553 1708
CONECT 1926 1496 1925
CONECT 1946 1944 2442
CONECT 2302 347 2303 2313
CONECT 2303 2302 2304 2310
CONECT 2304 2303 2305 2311
CONECT 2305 2304 2306 2312
CONECT 2306 2305 2307 2313
CONECT 2307 2306 2314
CONECT 2308 2309 2310 2315
CONECT 2309 2308
```

FIG. 53-120

CONECT 2311 2304
CONECT 2312 2305
CONECT 2313 2302 2306
CONECT 2314 2307
CONECT 2315 2308
CONECT 2316 628 2317 2327
CONECT 2317 2316 2318 2324
CONECT 2318 2317 2319 2325
CONECT 2319 2318 2320 2326
CONECT 2320 2319 2321 2327
CONECT 2321 2320 2328
CONECT 2322 2323 2324 2329
CONECT 2323 2322
CONECT 2324 2317 2322
CONECT 2325 2318
CONECT 2326 2319
CONECT 2327 2316 2320
CONECT 2328 2321 2456
CONECT 2329 2322
CONECT 2330 828 2331 2341
CONECT 2331 2330 2332 2338
CONECT 2332 2331 2333 2339
CONECT 2333 2332 2334 2340
CONECT 2334 2333 2335 2341
CONECT 2335 2334 2342
CONECT 2336 2337 2338 2343
CONECT 2337 2336
CONECT 2338 2331 2336
CONECT 2339 2332
CONECT 2340 2333
CONECT 2341 2330 2334
CONECT 2342 2335
CONECT 2343 2336
CONECT 2344 932 2345 2355
CONECT 2345 2344 2346 2352
CONECT 2346 2345 2347 2353
CONECT 2347 2346 2348 2354
CONECT 2348 2347 2349 2355
CONECT 2349 2348 2356
CONECT 2350 2351 2352 2357
CONECT 2351 2350
CONECT 2352 2345 2350
CONECT 2353 2346
CONECT 2354 2347
CONECT 2355 2344 2348
CONECT 2356 2349
CONECT 2357 2350
CONECT 2358 1035 2359 2369
CONECT 2359 2358 2360 2366
CONECT 2360 2359 2361 2367
CONECT 2361 2360 2362 2368
CONECT 2362 2361 2363 2369
CONECT 2363 2362 2370
CONECT 2364 2365 2366 2371
CONECT 2365 2364
CONECT 2366 2359 2364
CONECT 2367 2360
CONECT 2368 2361
CONECT 2369 2358 2362
CONECT 2370 2363
CONECT 2371 2364
CONECT 2372 1080 2373 2383
CONECT 2373 2372 2374 2380
CONECT 2374 2373 2375 2381
CONECT 2375 2374 2376 2382
CONECT 2376 2375 2377 2383
CONECT 2377 2376 2384
CONECT 2378 2379 2380 2385
CONECT 2379 2378
CONECT 2380 2373 2378

FIG. 53-121

CONECT 2382 2375
CONECT 2383 2372 2376
CONECT 2384 2377 2466
CONECT 2385 2378
CONECT 2386 1130 2387 2397
CONECT 2387 2386 2388 2394
CONECT 2388 2387 2389 2395
CONECT 2389 2388 2390 2396
CONECT 2390 2389 2391 2397
CONECT 2391 2390 2398
CONECT 2392 2393 2394 2399
CONECT 2393 2392
CONECT 2394 2387 2392
CONECT 2395 2388
CONECT 2396 2389
CONECT 2397 2386 2390
CONECT 2398 2391
CONECT 2399 2392
CONECT 2400 1191 2401 2411
CONECT 2401 2400 2402 2408
CONECT 2402 2401 2403 2409
CONECT 2403 2402 2404 2410
CONECT 2404 2403 2405 2411
CONECT 2405 2404 2412
CONECT 2406 2407 2408 2413
CONECT 2407 2406
CONECT 2408 2401 2406
CONECT 2409 2402
CONECT 2410 2403
CONECT 2411 2400 2404
CONECT 2412 2405
CONECT 2413 2406
CONECT 2414 1561 2415 2425
CONECT 2415 2414 2416 2422
CONECT 2416 2415 2417 2423
CONECT 2417 2416 2418 2424
CONECT 2418 2417 2419 2425
CONECT 2419 2418 2426
CONECT 2420 2421 2422 2427
CONECT 2421 2420
CONECT 2422 2415 2420
CONECT 2423 2416
CONECT 2424 2417
CONECT 2425 2414 2418
CONECT 2426 2419
CONECT 2427 2420
CONECT 2428 1610 2429 2439
CONECT 2429 2428 2430 2436
CONECT 2430 2429 2431 2437
CONECT 2431 2430 2432 2438
CONECT 2432 2431 2433 2439
CONECT 2433 2432 2440
CONECT 2434 2435 2436 2441
CONECT 2435 2434
CONECT 2436 2429 2434
CONECT 2437 2430
CONECT 2438 2431
CONECT 2439 2428 2432
CONECT 2440 2433 2476
CONECT 2441 2434
CONECT 2442 1946 2443 2453
CONECT 2443 2442 2444 2450
CONECT 2444 2443 2445 2451
CONECT 2445 2444 2446 2452
CONECT 2446 2445 2447 2453
CONECT 2447 2446 2454
CONECT 2448 2449 2450 2455
CONECT 2449 2448
CONECT 2450 2443 2448
CONECT 2451 2444

FIG. 53-122

```
CONECT 2453 2442 2446
CONECT 2454 2447 2486
CONECT 2455 2448
CONECT 2456 2328 2457 2465
CONECT 2457 2456 2458 2462
CONECT 2458 2457 2459 2463
CONECT 2459 2458 2460 2464
CONECT 2460 2459 2461 2465
CONECT 2461 2460
CONECT 2462 2457
CONECT 2463 2458
CONECT 2464 2459
CONECT 2465 2456 2460
CONECT 2466 2384 2467 2475
CONECT 2467 2466 2468 2472
CONECT 2468 2467 2469 2473
CONECT 2469 2468 2470 2474
CONECT 2470 2469 2471 2475
CONECT 2471 2470
CONECT 2472 2467
CONECT 2473 2468
CONECT 2474 2469
CONECT 2475 2466 2470
CONECT 2476 2440 2477 2485
CONECT 2477 2476 2478 2482
CONECT 2478 2477 2479 2483
CONECT 2479 2478 2480 2484
CONECT 2480 2479 2481 2485
CONECT 2481 2480
CONECT 2482 2477
CONECT 2483 2478
CONECT 2484 2479
CONECT 2485 2476 2480
CONECT 2486 2454 2487 2495
CONECT 2487 2486 2488 2492
CONECT 2488 2487 2489 2493
CONECT 2489 2488 2490 2494
CONECT 2490 2489 2491 2495
CONECT 2491 2490
CONECT 2492 2487
CONECT 2493 2488
CONECT 2494 2489
CONECT 2495 2486 2490
CONECT 2613 2612 3162
CONECT 3162 2613 3161
CONECT 3506 3505 3725
CONECT 3725 3506 3724
CONECT 4073 4072 4562
CONECT 4562 4073 4561
CONECT 4942 4941 5421
CONECT 5421 4942 5420
CONECT 5711 5710 6304
CONECT 6304 5711 6303
CONECT 6719 6718 7133
CONECT 7133 6719 7132
MASTER    231  0  15  13  75  0  1  6 7877  4 231  75
END
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FIG. 54A

Detailed here is a list of all the contacts between gp120 (designed here as molecule A) and CD4 (designated here as molecule B). The model is 7s_pb6 (from 26dec97).

Hydrogen bonds

	donor atom			acceptor atom		distance		
A	/A0125-LEU	N	B	/B1064-GLN	OE1	3.71MS	-1 7.14154.7 2.78111.6 111.5	48
B	/B1029-LYS	NZ	A	/A0279-ASP	OD2	2.75SS	-111.18152.4 1.81157.8 148.6	131
B	/B1029-LYS	NZ	A	/A0280-ASN	OD1	3.16SS	-110.25102.0 2.78145.4 141.4	134
A	/A0280-ASN	ND2	B	/B1033-GLN	O	2.71SM	-1 7.94151.6 1.79151.4 156.3	135
B	/B1052-ASN	ND2	A	/A0365-SER	O	2.97SM	-1 7.55135.0 2.18100.5 108.2	198
B	/B1046-LYS	N	A	/A0366-GLY	O	3.31MM	-1 4.90170.1 2.32114.3 112.0	199
A	/A0368-ASP	N	B	/B1044-LEU	O	3.44MM	-1 5.66143.5 2.59123.5 131.5	200
B	/B1059-ARG	NH2	A	/A0368-ASP	OD1	2.48SS	-111.53126.4 1.75 92.2 107.9	202
B	/B1044-LEU	N	A	/A0368-ASP	OD2	3.32MS	-1 5.66160.6 2.36 92.8 95.9	203
B	/B1059-ARG	NH1	A	/A0368-ASP	OD2	2.78SS	-111.53150.6 1.86132.1 121.9	204
B	/B1042-SER	OG	A	/A0427-TRP	O	3.42SM	-1 5.39178.3 2.42101.0 100.7	245
B	/B1025-GLN	NE2	A	/A0474-ASP	OD2	3.04SS	-1 9.17117.4 2.45 96.8 111.5	267

Van der Waals contacts

	donor atom			acceptor atom		distance			
B	/B1060-SER	CA	A	/A0123-THR	OG1	4.12MS	-1 5.83 -1.0-1.00 -1.0	99.7	1468
B	/B1063-ASP	OD2	A	/A0123-THR	O	3.97SM	-1 8.60 -1.0-1.00 -1.0	154.0	1484
B	/B1064-GLN	OE1	A	/A0125-LEU	N	3.71SM	-1 7.14 -1.0-1.00 -1.0	98.5	1535
B	/B1064-GLN	OE1	A	/A0125-LEU	CA	4.18SM	-1 7.14 -1.0-1.00 -1.0	56.9	1539
B	/B1060-SER	O	A	/A0125-LEU	CB	3.65MS	-1 6.24 -1.0-1.00 -1.0	54.9	1542
B	/B1064-GLN	CG	A	/A0125-LEU	CB	4.14SS	-1 7.14 -1.0-1.00 -1.0	113.5	1543
B	/B1064-GLN	CD	A	/A0125-LEU	CB	4.09SS	-1 7.14 -1.0-1.00 -1.0	101.0	1544
B	/B1064-GLN	OE1	A	/A0125-LEU	CB	3.58SS	-1 7.14 -1.0-1.00 -1.0	102.1	1545
B	/B1060-SER	CB	A	/A0125-LEU	CG	3.83SS	-1 6.24 -1.0-1.00 -1.0	62.6	1548
B	/B1060-SER	C	A	/A0125-LEU	CG	3.58MS	-1 6.24 -1.0-1.00 -1.0	74.4	1549
B	/B1060-SER	O	A	/A0125-LEU	CG	3.04MS	-1 6.24 -1.0-1.00 -1.0	69.7	1550
B	/B1061-LEU	CD2	A	/A0125-LEU	CG	3.72SS	-1 6.32 -1.0-1.00 -1.0	79.7	1551
B	/B1061-LEU	CD2	A	/A0125-LEU	CD1	3.76SS	-1 6.32 -1.0-1.00 -1.0	76.8	1554
B	/B1060-SER	CA	A	/A0125-LEU	CD2	3.73MS	-1 6.24 -1.0-1.00 -1.0	98.6	1556
B	/B1060-SER	CB	A	/A0125-LEU	CD2	3.41SS	-1 6.24 -1.0-1.00 -1.0	94.1	1557
B	/B1060-SER	C	A	/A0125-LEU	CD2	3.49MS	-1 6.24 -1.0-1.00 -1.0	80.8	1558
B	/B1060-SER	O	A	/A0125-LEU	CD2	2.89MS	-1 6.24 -1.0-1.00 -1.0	80.7	1559
B	/B1029-LYS	NZ	A	/A0279-ASP	CG	3.87SS	-111.18143.9 3.01125.2	21.7	4270
B	/B1027-HIS	CE1	A	/A0279-ASP	OD1	3.89SS	-110.91 -1.0-1.00 -1.0	115.1	4278
B	/B1029-LYS	CE	A	/A0279-ASP	OD2	3.86SS	-111.18 -1.0-1.00 -1.0	157.5	4288
B	/B1029-LYS	NZ	A	/A0279-ASP	OD2	2.75SS	-111.18152.4 1.81157.8	148.6	4289
B	/B1035-LYS	CD	A	/A0280-ASN	CB	3.84SS	-1 7.81 -1.0-1.00 -1.0	60.0	4321
B	/B1029-LYS	CE	A	/A0280-ASN	CG	4.10SS	-110.25 -1.0-1.00 -1.0	25.5	4326
B	/B1029-LYS	NZ	A	/A0280-ASN	CG	4.19SS	-110.25101.9 3.87121.4	28.0	4327
B	/B1033-GLN	O	A	/A0280-ASN	CG	3.70MS	-1 7.94 -1.0-1.00 -1.0	34.4	4328
B	/B1035-LYS	CD	A	/A0280-ASN	CG	3.35SS	-1 7.81 -1.0-1.00 -1.0	72.3	4329
B	/B1029-LYS	CE	A	/A0280-ASN	OD1	3.03SS	-110.25 -1.0-1.00 -1.0	144.3	4335
B	/B1029-LYS	NZ	A	/A0280-ASN	OD1	3.16SS	-110.25102.0 2.78145.4	141.4	4336
B	/B1033-GLN	O	A	/A0280-ASN	OD1	3.89MS	-1 7.94 -1.0-1.00 -1.0	71.8	4337
B	/B1035-LYS	CG	A	/A0280-ASN	OD1	3.77SS	-1 7.81 -1.0-1.00 -1.0	105.2	4338
B	/B1035-LYS	CD	A	/A0280-ASN	OD1	3.20SS	-1 7.81 -1.0-1.00 -1.0	86.0	4339
B	/B1035-LYS	CE	A	/A0280-ASN	OD1	4.11SS	-1 7.81 -1.0-1.00 -1.0	87.5	4340
B	/B1033-GLN	CB	A	/A0280-ASN	ND2	4.13SS	-1 7.94 -1.0-1.00 -1.0	132.0	4343
B	/B1033-GLN	C	A	/A0280-ASN	ND2	3.87MS	-1 7.94 -1.0-1.00 -1.0	134.5	4344
B	/B1033-GLN	O	A	/A0280-ASN	ND2	2.71MS	-1 7.94 -1.0-1.00 -1.0	129.6	4345
B	/B1035-LYS	CD	A	/A0280-ASN	ND2	3.85SS	-1 7.81 -1.0-1.00 -1.0	58.2	4346
B	/B1035-LYS	CD	A	/A0280-ASN	C	3.83SM	-1 7.81 -1.0-1.00 -1.0	75.4	4352
B	/B1035-LYS	CE	A	/A0280-ASN	C	3.57SM	-1 7.81 -1.0-1.00 -1.0	53.2	4353

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FIG. 54B

B	/B1035-LYS	CE	A	/A0280-ASN	O	3.00SM	-1 7.81 -1.0-1.00 -1.0	107.7	4362
B	/B1035-LYS	CD	A	/A0281-ALA	N	4.03SM	-1 7.00 -1.0-1.00 -1.0	71.7	4365
B	/B1035-LYS	CE	A	/A0281-ALA	N	3.94SM	-1 7.00 -1.0-1.00 -1.0	64.4	4366
B	/B1035-LYS	CD	A	/A0281-ALA	CA	4.16SM	-1 7.00 -1.0-1.00 -1.0	74.8	4368
B	/B1035-LYS	CE	A	/A0281-ALA	CA	3.80SM	-1 7.00 -1.0-1.00 -1.0	84.3	4369
B	/B1027-HIS	CG	A	/A0281-ALA	CB	3.57SS	-1 7.00 -1.0-1.00 -1.0	147.8	4372
B	/B1027-HIS	CD2	A	/A0281-ALA	CB	3.64SS	-1 7.00 -1.0-1.00 -1.0	139.6	4373
B	/B1027-HIS	ND1	A	/A0281-ALA	CB	3.31SS	-1 7.00 61.5 3.67160.4	168.7	4374
B	/B1027-HIS	CE1	A	/A0281-ALA	CB	3.24SS	-1 7.00 -1.0-1.00 -1.0	165.4	4375
B	/B1027-HIS	NE2	A	/A0281-ALA	CB	3.44SS	-1 7.00 56.4 3.89134.4	146.1	4376
B	/B1029-LYS	CE	A	/A0281-ALA	CB	4.02SS	-1 9.11 -1.0-1.00 -1.0	112.9	4377
B	/B1029-LYS	NZ	A	/A0281-ALA	CB	4.09SS	-1 9.11125.9 3.41105.0	112.6	4378
B	/B1040-GLN	CD	A	/A0283-THR	OG1	3.78SS	-1 9.11 -1.0-1.00 -1.0	172.3	4419
B	/B1040-GLN	OE1	A	/A0283-THR	OG1	3.38SS	-1 9.11 -1.0-1.00 -1.0	164.0	4420
B	/B1040-GLN	NE2	A	/A0283-THR	OG1	3.67SS	-1 9.11110.8 3.19139.9	152.1	4421
B	/B1046-LYS	O	A	/A0365-SER	CA	3.92MM	-1 5.83 -1.0-1.00 -1.0	40.5	6411
B	/B1046-LYS	C	A	/A0365-SER	CB	3.76MS	-1 5.83 -1.0-1.00 -1.0	111.4	6414
B	/B1046-LYS	O	A	/A0365-SER	CB	2.93MS	-1 5.83 -1.0-1.00 -1.0	110.5	6415
B	/B1047-GLY	N	A	/A0365-SER	CB	4.10MS	-1 5.10 20.9 5.02146.7	98.6	6416
B	/B1047-GLY	CA	A	/A0365-SER	CB	3.62MS	-1 5.10 -1.0-1.00 -1.0	79.3	6417
B	/B1047-GLY	C	A	/A0365-SER	CB	3.24MS	-1 5.10 -1.0-1.00 -1.0	80.2	6418
B	/B1047-GLY	O	A	/A0365-SER	CB	3.21MS	-1 5.10 -1.0-1.00 -1.0	100.1	6419
B	/B1048-PRO	N	A	/A0365-SER	CB	3.71MS	-1 5.39 -1.0-1.00 -1.0	63.0	6420
B	/B1052-ASN	ND2	A	/A0365-SER	CB	3.93SS	-1 7.55106.8 3.52156.0	91.9	6421
B	/B1046-LYS	O	A	/A0365-SER	OG	3.67MS	-1 5.83 -1.0-1.00 -1.0	48.4	6428
B	/B1047-GLY	CA	A	/A0365-SER	OG	3.64MS	-1 5.10 -1.0-1.00 -1.0	78.2	6429
B	/B1047-GLY	C	A	/A0365-SER	OG	3.31MS	-1 5.10 -1.0-1.00 -1.0	74.9	6430
B	/B1047-GLY	O	A	/A0365-SER	OG	3.73MS	-1 5.10 -1.0-1.00 -1.0	58.0	6431
B	/B1048-PRO	N	A	/A0365-SER	OG	3.32MS	-1 5.39 -1.0-1.00 -1.0	94.6	6432
B	/B1048-PRO	CD	A	/A0365-SER	OG	3.43SS	-1 5.39 -1.0-1.00 -1.0	118.0	6433
B	/B1048-PRO	CA	A	/A0365-SER	OG	3.90MS	-1 5.39 -1.0-1.00 -1.0	95.1	6434
B	/B1048-PRO	CG	A	/A0365-SER	OG	3.38SS	-1 5.39 -1.0-1.00 -1.0	132.0	6435
B	/B1046-LYS	O	A	/A0365-SER	C	3.93MM	-1 5.83 -1.0-1.00 -1.0	65.9	6438
B	/B1052-ASN	ND2	A	/A0365-SER	C	3.56SM	-1 7.55144.7 2.70115.1	52.5	6439
B	/B1052-ASN	CG	A	/A0365-SER	O	3.69SM	-1 7.55 -1.0-1.00 -1.0	127.2	6442
B	/B1052-ASN	OD1	A	/A0365-SER	O	3.71SM	-1 7.55 -1.0-1.00 -1.0	139.5	6443
B	/B1052-ASN	ND2	A	/A0365-SER	O	2.97SM	-1 7.55135.0 2.18100.5	108.2	6444
B	/B1046-LYS	O	A	/A0366-GLY	N	3.60MM	-1 4.90 -1.0-1.00 -1.0	94.4	6447
B	/B1052-ASN	ND2	A	/A0366-GLY	N	4.20SM	-1 7.21162.2 3.24 83.1	53.0	6448
B	/B1046-LYS	N	A	/A0366-GLY	C	3.94MM	-1 4.90150.1 3.04116.2	51.1	6454
B	/B1046-LYS	CB	A	/A0366-GLY	C	4.06SM	-1 4.90 -1.0-1.00 -1.0	84.8	6455
B	/B1045-THR	CA	A	/A0366-GLY	O	4.05MM	-1 6.16 -1.0-1.00 -1.0	130.3	6459
B	/B1045-THR	C	A	/A0366-GLY	O	4.19MM	-1 6.16 -1.0-1.00 -1.0	119.9	6460
B	/B1046-LYS	N	A	/A0366-GLY	O	3.31MM	-1 4.90170.1 2.32114.3	112.0	6461
B	/B1046-LYS	CA	A	/A0366-GLY	O	4.14MM	-1 4.90 -1.0-1.00 -1.0	99.2	6462
B	/B1046-LYS	CB	A	/A0366-GLY	O	4.13SM	-1 4.90 -1.0-1.00 -1.0	77.9	6463
B	/B1046-LYS	O	A	/A0366-GLY	O	3.67MM	-1 4.90 -1.0-1.00 -1.0	110.6	6464
B	/B1044-LEU	O	A	/A0367-GLY	CA	3.70MM	-1 5.29 -1.0-1.00 -1.0	92.0	6470
B	/B1044-LEU	O	A	/A0367-GLY	C	4.04MM	-1 5.29 -1.0-1.00 -1.0	54.3	6477
B	/B1044-LEU	O	A	/A0368-ASP	N	3.44MM	-1 5.66 -1.0-1.00 -1.0	107.4	6488
B	/B1043-PHE	CB	A	/A0368-ASP	CB	4.00SS	-1 5.83 -1.0-1.00 -1.0	80.4	6500
B	/B1043-PHE	CD1	A	/A0368-ASP	CB	3.89SS	-1 5.83 -1.0-1.00 -1.0	78.3	6501
B	/B1043-PHE	CA	A	/A0368-ASP	CG	4.07MS	-1 5.83 -1.0-1.00 -1.0	72.0	6507
B	/B1043-PHE	CB	A	/A0368-ASP	CG	4.03SS	-1 5.83 -1.0-1.00 -1.0	77.9	6508
B	/B1043-PHE	CD1	A	/A0368-ASP	CG	3.87SS	-1 5.83 -1.0-1.00 -1.0	49.1	6509
B	/B1044-LEU	N	A	/A0368-ASP	CG	3.67MS	-1 5.66157.3 2.72110.6	64.2	6510
B	/B1059-ARG	CZ	A	/A0368-ASP	CG	3.76SS	-111.53 -1.0-1.00 -1.0	60.7	6511
B	/B1059-ARG	NH1	A	/A0368-ASP	CG	3.60SS	-111.53131.6 2.86148.6	40.9	6512
B	/B1059-ARG	NH2	A	/A0368-ASP	CG	3.10SS	-111.53150.5 2.19148.5	49.6	6513
B	/B1043-PHE	CA	A	/A0368-ASP	OD1	3.88MS	-1 5.83 -1.0-1.00 -1.0	90.2	6519
B	/B1043-PHE	CB	A	/A0368-ASP	OD1	3.96SS	-1 5.83 -1.0-1.00 -1.0	84.2	6520
B	/B1043-PHE	CG	A	/A0368-ASP	OD1	4.04SS	-1 5.83 -1.0-1.00 -1.0	100.3	6521
B	/B1043-PHE	CD1	A	/A0368-ASP	OD1	3.20SS	-1 5.83 -1.0-1.00 -1.0	113.8	6522
B	/B1043-PHE	CE1	A	/A0368-ASP	OD1	4.08SS	-1 5.83 -1.0-1.00 -1.0	125.2	6523
B	/B1044-LEU	N	A	/A0368-ASP	OD1	4.08MS	-1 5.66152.1 3.17 57.9	62.0	6524
B	/B1059-ARG	CZ	A	/A0368-ASP	OD1	3.37SS	-111.53 -1.0-1.00 -1.0	98.4	6525

FIG. 54C

B	/B1059-ARG NH2	A	/A0368-ASP OD1	2.48SS	-111.53126.4 1.75 92.2	107.9	6527
B	/B1044-LEU N	A	/A0368-ASP OD2	3.32MS	-1 5.66160.6 2.36 92.8	95.9	6528
B	/B1044-LEU CA	A	/A0368-ASP OD2	3.92MS	-1 5.66 -1.0-1.00 -1.0	114.9	6529
B	/B1044-LEU CB	A	/A0368-ASP OD2	3.50SS	-1 5.66 -1.0-1.00 -1.0	137.6	6530
B	/B1044-LEU O	A	/A0368-ASP OD2	4.02MS	-1 5.66 -1.0-1.00 -1.0	98.2	6531
B	/B1059-ARG CZ	A	/A0368-ASP OD2	3.33SS	-111.53 -1.0-1.00 -1.0	100.1	6532
B	/B1059-ARG NH1	A	/A0368-ASP OD2	2.78SS	-111.53150.6 1.86132.1	121.9	6533
B	/B1059-ARG NH2	A	/A0368-ASP OD2	3.06SS	-111.53135.8 2.26 70.4	80.0	6534
B	/B1043-PHE CD1	A	/A0370-GLU CB	4.00SS	-1 7.48 -1.0-1.00 -1.0	86.6	6631
B	/B1043-PHE CE1	A	/A0370-GLU CB	3.62SS	-1 7.48 -1.0-1.00 -1.0	71.9	6632
B	/B1043-PHE CE2	A	/A0370-GLU CB	4.16SS	-1 7.48 -1.0-1.00 -1.0	97.5	6633
B	/B1043-PHE CZ	A	/A0370-GLU CB	3.71SS	-1 7.48 -1.0-1.00 -1.0	78.5	6634
B	/B1043-PHE CD1	A	/A0370-GLU CG	4.20SS	-1 7.48 -1.0-1.00 -1.0	72.1	6640
B	/B1043-PHE CE1	A	/A0370-GLU CG	3.46SS	-1 7.48 -1.0-1.00 -1.0	79.0	6641
B	/B1043-PHE CZ	A	/A0370-GLU CG	3.72SS	-1 7.48 -1.0-1.00 -1.0	77.7	6642
B	/B1043-PHE CD1	A	/A0370-GLU CD	4.02SS	-1 7.48 -1.0-1.00 -1.0	54.3	6651
B	/B1043-PHE CE1	A	/A0370-GLU CD	3.51SS	-1 7.48 -1.0-1.00 -1.0	73.6	6652
B	/B1043-PHE CD1	A	/A0370-GLU OE2	3.44SS	-1 7.48 -1.0-1.00 -1.0	108.6	6668
B	/B1043-PHE CE1	A	/A0370-GLU OE2	3.38SS	-1 7.48 -1.0-1.00 -1.0	85.6	6669
B	/B1044-LEU O	A	/A0371-ILE CB	4.04MS	-1 7.62 -1.0-1.00 -1.0	71.8	6695
B	/B1044-LEU O	A	/A0371-ILE CG2	4.02MS	-1 7.62 -1.0-1.00 -1.0	80.1	6700
B	/B1045-THR CG2	A	/A0371-ILE CG2	3.79SS	-1 7.07 -1.0-1.00 -1.0	113.2	6701
B	/B1043-PHE CB	A	/A0371-ILE CG1	3.23SS	-1 6.78 -1.0-1.00 -1.0	100.0	6704
B	/B1043-PHE CG	A	/A0371-ILE CG1	3.83SS	-1 6.78 -1.0-1.00 -1.0	86.6	6705
B	/B1043-PHE CD2	A	/A0371-ILE CG1	4.18SS	-1 6.78 -1.0-1.00 -1.0	67.3	6706
B	/B1044-LEU O	A	/A0371-ILE CG1	3.85MS	-1 7.62 -1.0-1.00 -1.0	86.2	6707
B	/B1043-PHE CB	A	/A0371-ILE CD1	3.79SS	-1 6.78 -1.0-1.00 -1.0	56.9	6713
B	/B1043-PHE CG	A	/A0371-ILE CD1	4.03SS	-1 6.78 -1.0-1.00 -1.0	71.4	6714
B	/B1043-PHE CD2	A	/A0371-ILE CD1	3.86SS	-1 6.78 -1.0-1.00 -1.0	91.5	6715
B	/B1043-PHE CE1	A	/A0425-ASN CA	4.18SM	-1 7.21 -1.0-1.00 -1.0	52.7	7996
B	/B1043-PHE CD1	A	/A0425-ASN CB	3.83SS	-1 7.21 -1.0-1.00 -1.0	118.6	8000
B	/B1043-PHE CE1	A	/A0425-ASN CB	3.47SS	-1 7.21 -1.0-1.00 -1.0	106.7	8001
B	/B1043-PHE CE1	A	/A0425-ASN C	3.63SM	-1 7.21 -1.0-1.00 -1.0	55.5	8013
B	/B1043-PHE CZ	A	/A0425-ASN C	4.17SM	-1 7.21 -1.0-1.00 -1.0	43.8	8014
B	/B1043-PHE CE1	A	/A0425-ASN O	3.10SM	-1 7.21 -1.0-1.00 -1.0	105.3	8019
B	/B1043-PHE CZ	A	/A0425-ASN O	3.38SM	-1 7.21 -1.0-1.00 -1.0	121.5	8020
B	/B1042-SER CB	A	/A0426-MET C	4.18SM	-1 6.71 -1.0-1.00 -1.0	26.9	8055
B	/B1043-PHE CE1	A	/A0426-MET C	3.99SM	-1 7.81 -1.0-1.00 -1.0	60.1	8056
B	/B1043-PHE CZ	A	/A0426-MET C	3.67SM	-1 7.81 -1.0-1.00 -1.0	71.0	8057
B	/B1042-SER CB	A	/A0426-MET O	3.13SM	-1 6.71 -1.0-1.00 -1.0	142.8	8063
B	/B1042-SER OG	A	/A0426-MET O	3.82SM	-1 6.71106.4 3.42108.3	122.6	8064
B	/B1043-PHE CE1	A	/A0426-MET O	3.54SM	-1 7.81 -1.0-1.00 -1.0	102.2	8065
B	/B1043-PHE CE2	A	/A0426-MET O	4.12SM	-1 7.81 -1.0-1.00 -1.0	97.5	8066
B	/B1043-PHE CZ	A	/A0426-MET O	3.47SM	-1 7.81 -1.0-1.00 -1.0	89.3	8067
B	/B1043-PHE CZ	A	/A0427-TRP N	3.74SM	-1 7.00 -1.0-1.00 -1.0	76.0	8075
B	/B1043-PHE CE2	A	/A0427-TRP CA	3.72SM	-1 7.00 -1.0-1.00 -1.0	73.6	8080
B	/B1043-PHE CZ	A	/A0427-TRP CA	3.67SM	-1 7.00 -1.0-1.00 -1.0	80.7	8081
B	/B1043-PHE CE2	A	/A0427-TRP CB	3.61SS	-1 7.00 -1.0-1.00 -1.0	82.2	8088
B	/B1043-PHE CZ	A	/A0427-TRP CB	3.75SS	-1 7.00 -1.0-1.00 -1.0	75.4	8089
B	/B1042-SER OG	A	/A0427-TRP C	3.84SM	-1 5.39165.6 2.86109.0	61.0	8137
B	/B1042-SER CB	A	/A0427-TRP O	4.10SM	-1 5.39 -1.0-1.00 -1.0	91.1	8142
B	/B1042-SER OG	A	/A0427-TRP O	3.42SM	-1 5.39178.3 2.42101.0	100.7	8143
B	/B1042-SER OG	A	/A0428-GLN C	3.93SM	-1 7.00144.1 3.08111.8	63.1	8161
B	/B1042-SER OG	A	/A0428-GLN O	4.11SM	-1 7.00124.7 3.45 62.8	73.2	8165
B	/B1042-SER OG	A	/A0429-LYS N	3.53SM	-1 5.57156.5 2.59101.3	69.4	8169
B	/B1042-SER OG	A	/A0429-LYS CA	3.31SM	-1 5.57151.2 2.40163.3	66.5	8172
B	/B1042-SER CB	A	/A0429-LYS C	3.65SM	-1 5.57 -1.0-1.00 -1.0	72.5	8185
B	/B1042-SER OG	A	/A0429-LYS C	3.05SM	-1 5.57171.0 2.05 95.9	86.1	8186
B	/B1042-SER CB	A	/A0429-LYS O	3.49SM	-1 5.57 -1.0-1.00 -1.0	87.7	8191
B	/B1042-SER OG	A	/A0429-LYS O	3.23SM	-1 5.57149.1 2.33 63.9	70.2	8192
B	/B1042-SER CB	A	/A0430-VAL N	3.88SM	-1 4.80 -1.0-1.00 -1.0	70.4	8197
B	/B1042-SER OG	A	/A0430-VAL N	3.43SM	-1 4.80162.4 2.47109.9	62.1	8198
B	/B1042-SER CB	A	/A0430-VAL CA	4.00SM	-1 4.80 -1.0-1.00 -1.0	74.7	8200
B	/B1042-SER OG	A	/A0430-VAL CA	4.06SM	-1 4.80137.8 3.27139.6	54.7	8201
B	/B1059-ARG CB	A	/A0430-VAL CG1	3.68SS	-1 6.78 -1.0-1.00 -1.0	135.4	8207
B	/B1059-ARG C	A	/A0430-VAL CG1	4.13MS	-1 6.78 -1.0-1.00 -1.0	121.7	8208

FIG. 54D

B	/B1042-SER	CA	A	/A0430-VAL	CG2	3.98MS	-1 4.80 -1.0-1.00 -1.0	127.6	8211
B	/B1042-SER	CB	A	/A0430-VAL	CG2	4.01SS	-1 4.80 -1.0-1.00 -1.0	106.6	8212
B	/B1042-SER	O	A	/A0430-VAL	CG2	3.94MS	-1 4.80 -1.0-1.00 -1.0	115.4	8213
B	/B1062-TRP	CE3	A	/A0430-VAL	CG2	3.38SS	-1 7.87 -1.0-1.00 -1.0	142.7	8214
B	/B1062-TRP	CZ3	A	/A0430-VAL	CG2	3.96SS	-1 7.87 -1.0-1.00 -1.0	143.2	8215
B	/B1035-LYS	CE	A	/A0455-THR	CG2	3.99SS	-110.54 -1.0-1.00 -1.0	133.1	8736
B	/B1035-LYS	NZ	A	/A0455-THR	CG2	3.54SS	-110.54135.4 2.74136.5	144.6	8737
B	/B1035-LYS	CD	A	/A0456-ARG	O	4.17SM	-1 9.59 -1.0-1.00 -1.0	155.2	8795
B	/B1035-LYS	CE	A	/A0456-ARG	O	3.84SM	-1 9.59 -1.0-1.00 -1.0	142.6	8796
B	/B1048-PRO	CG	A	/A0457-ASP	CG	3.74SS	-1 7.35 -1.0-1.00 -1.0	66.0	8817
B	/B1048-PRO	CG	A	/A0457-ASP	OD1	3.75SS	-1 7.35 -1.0-1.00 -1.0	80.0	8824
B	/B1048-PRO	CG	A	/A0457-ASP	OD2	3.43SS	-1 7.35 -1.0-1.00 -1.0	94.6	8832
B	/B1034-ILE	CD1	A	/A0458-GLY	C	4.05SM	-1 5.29 -1.0-1.00 -1.0	72.8	8847
B	/B1034-ILE	CD1	A	/A0458-GLY	O	3.87SM	-1 5.29 -1.0-1.00 -1.0	89.5	8854
B	/B1032-ASN	O	A	/A0459-GLY	N	3.61MM	-1 5.10 -1.0-1.00 -1.0	58.0	8858
B	/B1033-GLN	O	A	/A0459-GLY	N	4.14MM	-1 5.10 -1.0-1.00 -1.0	98.1	8859
B	/B1034-ILE	CD1	A	/A0459-GLY	N	4.05SM	-1 5.29 -1.0-1.00 -1.0	69.7	8860
B	/B1032-ASN	O	A	/A0459-GLY	CA	3.09MM	-1 5.10 -1.0-1.00 -1.0	98.6	8862
B	/B1034-ILE	CD1	A	/A0459-GLY	CA	3.80SM	-1 5.29 -1.0-1.00 -1.0	89.3	8863
B	/B1048-PRO	CG	A	/A0469-ARG	NE	3.83SS	-110.34 -1.0-1.00 -1.0	78.9	9135
B	/B1048-PRO	CG	A	/A0469-ARG	CZ	3.80SS	-110.34 -1.0-1.00 -1.0	58.9	9136
B	/B1048-PRO	CB	A	/A0469-ARG	NH2	3.73SS	-110.34 -1.0-1.00 -1.0	119.1	9137
B	/B1048-PRO	CG	A	/A0469-ARG	NH2	3.32SS	-110.34 -1.0-1.00 -1.0	101.1	9138
B	/B1040-GLN	CB	A	/A0472-GLY	O	3.40SM	-1 6.86 -1.0-1.00 -1.0	128.3	9178
B	/B1040-GLN	CG	A	/A0472-GLY	O	3.48SM	-1 6.86 -1.0-1.00 -1.0	136.2	9179
B	/B1040-GLN	CD	A	/A0472-GLY	O	4.14SM	-1 6.86 -1.0-1.00 -1.0	117.0	9180
B	/B1040-GLN	NE2	A	/A0472-GLY	O	4.00SM	-1 6.86120.2 3.40 92.5	99.1	9181
B	/B1040-GLN	CB	A	/A0473-GLY	CA	3.86SM	-1 4.58 -1.0-1.00 -1.0	92.8	9186
B	/B1040-GLN	O	A	/A0473-GLY	CA	3.30MM	-1 4.58 -1.0-1.00 -1.0	65.4	9187
B	/B1043-PHE	CD2	A	/A0473-GLY	CA	3.87SM	-1 6.00 -1.0-1.00 -1.0	96.6	9188
B	/B1040-GLN	C	A	/A0473-GLY	C	3.79MM	-1 4.58 -1.0-1.00 -1.0	79.1	9193
B	/B1040-GLN	O	A	/A0473-GLY	C	3.00MM	-1 4.58 -1.0-1.00 -1.0	87.0	9194
B	/B1040-GLN	C	A	/A0473-GLY	O	4.09MM	-1 4.58 -1.0-1.00 -1.0	67.4	9201
B	/B1040-GLN	O	A	/A0473-GLY	O	3.18MM	-1 4.58 -1.0-1.00 -1.0	70.2	9202
B	/B1043-PHE	CD2	A	/A0473-GLY	O	3.90SM	-1 6.00 -1.0-1.00 -1.0	101.1	9203
B	/B1043-PHE	CE2	A	/A0473-GLY	O	4.05SM	-1 6.00 -1.0-1.00 -1.0	115.8	9204
B	/B1040-GLN	CB	A	/A0474-ASP	N	4.09SM	-1 4.90 -1.0-1.00 -1.0	86.0	9208
B	/B1040-GLN	NE2	A	/A0474-ASP	N	3.62SM	-1 4.90153.2 2.70120.8	103.2	9209
B	/B1040-GLN	C	A	/A0474-ASP	N	3.78MM	-1 4.90 -1.0-1.00 -1.0	80.7	9210
B	/B1040-GLN	O	A	/A0474-ASP	N	3.39MM	-1 4.90 -1.0-1.00 -1.0	61.8	9211
B	/B1040-GLN	NE2	A	/A0474-ASP	CA	4.20SM	-1 4.90131.5 3.47129.6	55.0	9216
B	/B1040-GLN	C	A	/A0474-ASP	CA	4.17MM	-1 4.90 -1.0-1.00 -1.0	64.5	9217
B	/B1040-GLN	O	A	/A0474-ASP	CA	4.01MM	-1 4.90 -1.0-1.00 -1.0	54.9	9218
B	/B1025-GLN	NE2	A	/A0474-ASP	CB	3.76SS	-1 9.17131.5 3.02122.7	75.7	9222
B	/B1040-GLN	NE2	A	/A0474-ASP	CB	3.55SS	-1 4.90105.3 3.15148.9	104.4	9223
B	/B1025-GLN	NE2	A	/A0474-ASP	CG	3.69SS	-1 9.17138.5 2.88133.3	50.1	9232
B	/B1025-GLN	CD	A	/A0474-ASP	OD2	4.09SS	-1 9.17 -1.0-1.00 -1.0	118.2	9246
B	/B1025-GLN	NE2	A	/A0474-ASP	OD2	3.04SS	-1 9.17117.4 2.45 96.8	111.5	9247
B	/B1040-GLN	NE2	A	/A0477-ASP	OD2	4.10SS	-1 9.49144.4 3.25134.2	134.4	9372

FIG. 55A

Detailed here is a list of all the contacts between gp120 (designed here as molecule A) and the Fab 17b (the light chain is designated here as molecule C; the heavy chain is designated here as molecule D). The model is 7s_pb6 (from 26dec97).

Hydrogen bonds

	donor atom		acceptor atom	distance		
C	/C2094-TRP NE1	A	/A0119-CYS SG	3.37SS	-110.05119.2 2.76115.1 124.6	40
A	/A0121-LYS NZ	D	/D3055-LEU O	2.64SM	-1 8.31111.1 2.10 96.1 115.1	43
A	/A0202-THR OG1	D	/D3059-HIS NE2	2.76SS	-1 8.60179.9 1.76136.3 107.3	53
D	/D3059-HIS NE2	A	/A0202-THR OG1	2.76SS	-1 8.60132.4 1.99103.7 110.1	54
A	/A0419-ARG NH1	D	/D3106-GLU OE1	2.76SS	-1 8.89138.6 1.93139.5 131.5	236
A	/A0419-ARG NH2	D	/D3106-GLU OE1	2.94SS	-1 8.89131.6 2.18122.8 121.6	237
A	/A0422-GLN N	D	/D3107-GLY O	2.84MM	-1 5.48155.6 1.90126.3 131.0	238
D	/D3109-TYR N	A	/A0422-GLN OE1	2.73MS	-1 6.08159.9 1.77161.2 156.1	239
A	/A0423-ILE N	D	/D3107-GLY O	2.89MM	-1 4.58165.6 1.91136.9 141.7	241

Van der Waals contacts

	donor atom		acceptor atom	distance		
C	/C2094-TRP CE2	A	/A0119-CYS SG	4.08SS	-110.05 -1.0-1.00 -1.0 115.4	1319
C	/C2094-TRP CD1	A	/A0119-CYS SG	4.16SS	-110.05 -1.0-1.00 -1.0 141.5	1320
C	/C2094-TRP NE1	A	/A0119-CYS SG	3.37SS	-110.05119.2 2.76115.1 124.6	1321
C	/C2094-TRP CE2	A	/A0202-THR CG2	4.19SS	-1 8.37 -1.0-1.00 -1.0 149.8	1802
C	/C2094-TRP NE1	A	/A0202-THR CG2	3.48SS	-1 8.37118.7 2.89131.0 145.6	1803
C	/C2095-PRO CA	A	/A0202-THR CG2	4.14MS	-1 6.48 -1.0-1.00 -1.0 148.5	1804
C	/C2095-PRO CB	A	/A0202-THR CG2	3.65SS	-1 6.48 -1.0-1.00 -1.0 127.3	1805
C	/C2095-PRO CG	A	/A0202-THR CG2	3.31SS	-1 6.48 -1.0-1.00 -1.0 116.7	1806
C	/C2095-PRO CG	A	/A0202-THR O	4.06SM	-1 6.48 -1.0-1.00 -1.0 113.1	1817
C	/C2094-TRP CD1	A	/A0203-GLN O	3.41SM	-1 8.00 -1.0-1.00 -1.0 135.7	1841
C	/C2094-TRP NE1	A	/A0203-GLN O	3.49SM	-1 8.00112.3 2.98147.4 149.2	1842
C	/C2094-TRP CD1	A	/A0205-CYS N	4.12SM	-1 7.42 -1.0-1.00 -1.0 110.8	1865
C	/C2094-TRP CZ2	A	/A0434-MET CE	3.88SS	-112.65 -1.0-1.00 -1.0 160.1	8276
C	/C2094-TRP CH2	A	/A0434-MET CE	3.86SS	-112.65 -1.0-1.00 -1.0 140.7	8277
D	/D3055-LEU CB	A	/A0121-LYS CD	4.13SS	-1 8.31 -1.0-1.00 -1.0 79.8	1380
D	/D3055-LEU O	A	/A0121-LYS CD	3.87MS	-1 8.31 -1.0-1.00 -1.0 77.5	1381
D	/D3057-VAL CG1	A	/A0121-LYS CD	3.85SS	-1 9.06 -1.0-1.00 -1.0 109.0	1382
D	/D3055-LEU CB	A	/A0121-LYS CE	4.14SS	-1 8.31 -1.0-1.00 -1.0 57.4	1383
D	/D3055-LEU CG	A	/A0121-LYS CE	4.09SS	-1 8.31 -1.0-1.00 -1.0 74.0	1384
D	/D3055-LEU O	A	/A0121-LYS CE	3.83MS	-1 8.31 -1.0-1.00 -1.0 29.5	1385
D	/D3055-LEU CA	A	/A0121-LYS NZ	3.30MS	-1 8.31 -1.0-1.00 -1.0 126.8	1386
D	/D3055-LEU CB	A	/A0121-LYS NZ	3.56SS	-1 8.31 -1.0-1.00 -1.0 102.0	1387
D	/D3055-LEU CG	A	/A0121-LYS NZ	3.94SS	-1 8.31 -1.0-1.00 -1.0 84.8	1388
D	/D3055-LEU C	A	/A0121-LYS NZ	3.36MS	-1 8.31 -1.0-1.00 -1.0 136.7	1389
D	/D3055-LEU O	A	/A0121-LYS NZ	2.64MS	-1 8.31 -1.0-1.00 -1.0 134.4	1390
D	/D3057-VAL CG1	A	/A0200-VAL CB	3.75SS	-1 7.35 -1.0-1.00 -1.0 71.3	1745
D	/D3057-VAL CG1	A	/A0200-VAL CG1	3.57SS	-1 7.35 -1.0-1.00 -1.0 84.9	1747
D	/D3059-HIS CD2	A	/A0202-THR CB	3.94SS	-1 8.60 -1.0-1.00 -1.0 56.4	1792
D	/D3059-HIS NE2	A	/A0202-THR CB	3.52SS	-1 8.60138.2 2.71119.7 47.4	1793
D	/D3059-HIS CD2	A	/A0202-THR OG1	3.44SS	-1 8.60 -1.0-1.00 -1.0 99.6	1796
D	/D3059-HIS NE2	A	/A0202-THR OG1	2.76SS	-1 8.60132.4 1.99103.7 110.1	1797
D	/D3059-HIS CE1	A	/A0202-THR OG1	3.82SS	-1 8.60 -1.0-1.00 -1.0 122.6	1798
D	/D3059-HIS CD2	A	/A0202-THR CG2	3.35SS	-1 8.60 -1.0-1.00 -1.0 101.3	1807
D	/D3059-HIS NE2	A	/A0202-THR CG2	3.12SS	-1 8.60121.9 2.47 81.9 92.2	1808
D	/D3106-GLU O	A	/A0419-ARG CD	4.00MS	-1 8.89 -1.0-1.00 -1.0 68.2	7757
D	/D3106-GLU O	A	/A0419-ARG NE	3.72MS	-1 8.89 -1.0-1.00 -1.0 90.2	7758
D	/D3106-GLU CB	A	/A0419-ARG CZ	3.76SS	-1 8.89 -1.0-1.00 -1.0 79.6	7759
D	/D3106-GLU CD	A	/A0419-ARG CZ	4.09SS	-1 8.89 -1.0-1.00 -1.0 64.2	7760
D	/D3106-GLU OE1	A	/A0419-ARG CZ	3.23SS	-1 8.89 -1.0-1.00 -1.0 57.6	7761

FIG. 55B

D	/D3106-GLU CB	A	/A0419-ARG NH1	3.79SS	-1	8.89	-1.0-1.00	-1.0	78.6	7763
D	/D3106-GLU CG	A	/A0419-ARG NH1	3.90SS	-1	8.89	-1.0-1.00	-1.0	98.1	7764
D	/D3106-GLU CD	A	/A0419-ARG NH1	3.71SS	-1	8.89	-1.0-1.00	-1.0	97.0	7765
D	/D3106-GLU OE1	A	/A0419-ARG NH1	2.76SS	-1	8.89	-1.0-1.00	-1.0	98.4	7766
D	/D3106-GLU CB	A	/A0419-ARG NH2	3.76SS	-1	8.89	-1.0-1.00	-1.0	80.0	7767
D	/D3106-GLU CD	A	/A0419-ARG NH2	3.75SS	-1	8.89	-1.0-1.00	-1.0	95.1	7768
D	/D3106-GLU OE1	A	/A0419-ARG NH2	2.94SS	-1	8.89	-1.0-1.00	-1.0	90.3	7769
D	/D3108-GLU CB	A	/A0419-ARG NH2	3.48SS	-1	8.89	-1.0-1.00	-1.0	119.9	7770
D	/D3108-GLU CG	A	/A0419-ARG NH2	4.07SS	-1	8.89	-1.0-1.00	-1.0	131.1	7771
D	/D3108-GLU CD	A	/A0419-ARG NH2	3.54SS	-1	8.89	-1.0-1.00	-1.0	144.5	7772
D	/D3108-GLU OE1	A	/A0419-ARG NH2	3.89SS	-1	8.89	-1.0-1.00	-1.0	163.1	7773
D	/D3108-GLU OE2	A	/A0419-ARG NH2	3.40SS	-1	8.89	-1.0-1.00	-1.0	130.5	7774
D	/D3107-GLY C	A	/A0421-LYS CA	4.19MM	-1	4.58	-1.0-1.00	-1.0	72.9	7812
D	/D3107-GLY O	A	/A0421-LYS CA	3.94MM	-1	4.58	-1.0-1.00	-1.0	74.7	7813
D	/D3106-GLU O	A	/A0421-LYS CB	4.03MS	-1	7.00	-1.0-1.00	-1.0	45.2	7817
D	/D3107-GLY CA	A	/A0421-LYS CB	3.94MS	-1	4.58	-1.0-1.00	-1.0	83.7	7818
D	/D3107-GLY C	A	/A0421-LYS CB	4.02MS	-1	4.58	-1.0-1.00	-1.0	85.8	7819
D	/D3107-GLY O	A	/A0421-LYS CB	3.98MS	-1	4.58	-1.0-1.00	-1.0	77.1	7820
D	/D3106-GLU C	A	/A0421-LYS CG	4.17MS	-1	7.00	-1.0-1.00	-1.0	66.3	7823
D	/D3106-GLU O	A	/A0421-LYS CG	3.16MS	-1	7.00	-1.0-1.00	-1.0	72.9	7824
D	/D3107-GLY CA	A	/A0421-LYS CG	4.06MS	-1	4.58	-1.0-1.00	-1.0	73.7	7825
D	/D3106-GLU C	A	/A0421-LYS CD	3.82MS	-1	7.00	-1.0-1.00	-1.0	79.4	7826
D	/D3106-GLU O	A	/A0421-LYS CD	3.07MS	-1	7.00	-1.0-1.00	-1.0	75.7	7827
D	/D3107-GLY CA	A	/A0421-LYS CD	3.91MS	-1	4.58	-1.0-1.00	-1.0	84.5	7828
D	/D3106-GLU C	A	/A0421-LYS CE	3.85MS	-1	7.00	-1.0-1.00	-1.0	77.8	7829
D	/D3106-GLU O	A	/A0421-LYS CE	3.07MS	-1	7.00	-1.0-1.00	-1.0	75.7	7830
D	/D3106-GLU C	A	/A0421-LYS NZ	3.87MS	-1	7.00	-1.0-1.00	-1.0	78.2	7831
D	/D3106-GLU O	A	/A0421-LYS NZ	3.53MS	-1	7.00	-1.0-1.00	-1.0	60.2	7832
D	/D3107-GLY O	A	/A0421-LYS C	3.83MM	-1	4.58	-1.0-1.00	-1.0	34.8	7839
D	/D3107-GLY C	A	/A0422-GLN N	3.76MM	-1	5.48	-1.0-1.00	-1.0	115.7	7851
D	/D3107-GLY O	A	/A0422-GLN N	2.84MM	-1	5.48	-1.0-1.00	-1.0	106.7	7852
D	/D3107-GLY O	A	/A0422-GLN CA	3.54MM	-1	5.48	-1.0-1.00	-1.0	50.1	7856
D	/D3107-GLY O	A	/A0422-GLN CB	3.75MS	-1	5.48	-1.0-1.00	-1.0	70.5	7862
D	/D3109-TYR O	A	/A0422-GLN CG	4.19MS	-1	6.08	-1.0-1.00	-1.0	71.1	7867
D	/D3109-TYR N	A	/A0422-GLN CD	3.89MS	-1	6.08154.5	2.96123.6		16.5	7868
D	/D3109-TYR O	A	/A0422-GLN CD	3.97MS	-1	6.08	-1.0-1.00	-1.0	39.7	7869
D	/D3108-GLU CA	A	/A0422-GLN OE1	3.65MS	-1	5.39	-1.0-1.00	-1.0	121.3	7870
D	/D3108-GLU CG	A	/A0422-GLN OE1	3.98SS	-1	5.39	-1.0-1.00	-1.0	126.1	7871
D	/D3108-GLU C	A	/A0422-GLN OE1	3.63MS	-1	5.39	-1.0-1.00	-1.0	141.7	7872
D	/D3109-TYR N	A	/A0422-GLN OE1	2.73MS	-1	6.08159.9	1.77161.2		156.1	7873
D	/D3109-TYR CA	A	/A0422-GLN OE1	3.57MS	-1	6.08	-1.0-1.00	-1.0	157.4	7874
D	/D3109-TYR C	A	/A0422-GLN OE1	3.34MS	-1	6.08	-1.0-1.00	-1.0	147.2	7875
D	/D3109-TYR O	A	/A0422-GLN OE1	3.13MS	-1	6.08	-1.0-1.00	-1.0	125.8	7876
D	/D3110-ASP N	A	/A0422-GLN OE1	4.12MS	-1	8.19	50.6	4.68157.4	148.4	7877
D	/D3107-GLY O	A	/A0422-GLN C	3.68MM	-1	5.48	-1.0-1.00	-1.0	44.6	7887
D	/D3107-GLY C	A	/A0423-ILE N	3.93MM	-1	4.58	-1.0-1.00	-1.0	112.0	7906
D	/D3107-GLY O	A	/A0423-ILE N	2.89MM	-1	4.58	-1.0-1.00	-1.0	116.5	7907
D	/D3107-GLY O	A	/A0423-ILE CA	3.85MM	-1	4.58	-1.0-1.00	-1.0	40.3	7911
D	/D3103-GLU OE2	A	/A0423-ILE CB	3.55SS	-1	8.19	-1.0-1.00	-1.0	72.3	7915
D	/D3107-GLY CA	A	/A0423-ILE CB	4.16MS	-1	4.58	-1.0-1.00	-1.0	91.1	7916
D	/D3107-GLY O	A	/A0423-ILE CB	3.77MS	-1	4.58	-1.0-1.00	-1.0	70.4	7917
D	/D3103-GLU OE2	A	/A0423-ILE CG2	4.13SS	-1	8.19	-1.0-1.00	-1.0	57.2	7925
D	/D3103-GLU OE2	A	/A0423-ILE CG1	3.42SS	-1	8.19	-1.0-1.00	-1.0	82.2	7927
D	/D3107-GLY O	A	/A0423-ILE CG1	3.56MS	-1	4.58	-1.0-1.00	-1.0	85.6	7928
D	/D3109-TYR CB	A	/A0423-ILE CG1	4.14SS	-1	7.14	-1.0-1.00	-1.0	82.8	7929
D	/D3107-GLY CA	A	/A0423-ILE O	3.80MM	-1	4.58	-1.0-1.00	-1.0	127.6	7943
D	/D3107-GLY O	A	/A0423-ILE O	4.15MM	-1	4.58	-1.0-1.00	-1.0	96.5	7944
D	/D3109-TYR CD1	A	/A0434-MET SD	3.83SS	-1	8.37	-1.0-1.00	-1.0	119.5	8274
D	/D3111-ASN ND2	A	/A0434-MET SD	3.36SS	-1	9.75121.6	2.73117.9		60.9	8275
D	/D3052-ILE CD1	A	/A0434-MET CE	4.03SS	-110.77		-1.0-1.00	-1.0	94.6	8278
D	/D3111-ASN ND2	A	/A0434-MET CE	2.94SS	-1	9.75100.8	2.58	74.8	87.1	8279
D	/D3110-ASP O	A	/A0437-PRO CD	3.90MS	-1	6.08	-1.0-1.00	-1.0	58.9	8341
D	/D3109-TYR O	A	/A0437-PRO CG	3.99MS	-1	7.55	-1.0-1.00	-1.0	110.3	8348
D	/D3110-ASP CA	A	/A0437-PRO CG	3.96MS	-1	6.08	-1.0-1.00	-1.0	125.3	8349

DECLARATION AND POWER OF ATTORNEY

As a below-named inventor, I hereby declare that:

My residence, post office address, and citizenship are as stated below next to my name.

I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:

Crystal Comprising Human Immunodeficiency Virus Envelope Glycoprotein GP120, Compounds Inhibiting CD4-gp120 Interaction, Compounds Inhibiting Chemokine Receptor gp-120 Interaction, Mimics of CD4 and gp120 Variants

the specification of which:
(check one)

__ is attached hereto.

X was filed on May 7, 2001 as

Application Serial No. 09/856,200

and was amended May 7, 2001 (if applicable)

I hereby state that I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose to the U.S. Patent and Trademark Office all information known to me to be material to patentability as defined in Title 37, Code of Federal Regulations, Section 1.56.

I hereby claim foreign priority benefits under Title 35, United States Code, Section 119 (a)-(d) or Section 365(b) of any foreign application(s) for patent or inventor's certificate, or Section 365(a) of any PCT international Application which designated at least one country other than the United States, listed below. I have also identified below any foreign application for patent or inventor's certificate, or PCT international Application having a filing date before that of the earliest application from which priority is claimed:

Prior Foreign Application(s)

Number	Country	Filing Date	Priority Claimed Yes	Priority Claimed No
PCT/US98/23905	PCT	November 10, 1998	X	

Declaration and Power of Attorney

I hereby claim the benefit under Title 35, United States Code, Section 119(e) of any United States provisional application(s) listed below:

Provisional Application No.	Filing Date	Status

I hereby claim the benefit under Title 35, United States Code, Section 120 of any United States Application(s), or Section 365(c) of any PCT International Application(s) designating the United States listed below. Insofar as this application discloses and claims subject matter in addition to that disclosed in any such prior Application in the manner provided by the first paragraph of Title 35, United States Code, Section 112, I acknowledge the duty to disclose to the United States Patent and Trademark Office all information known to me to be material to patentability as defined in Title 37, Code of Federal Regulations, Section 1.56, which became available between the filing date(s) of such prior Application(s) and the national or PCT international filing date of this application:

Application Serial No.	Filing Date	Status
08/966,987	November 10,1997	
08/967,403	November 10, 1997	
08/966,932	November 10, 1997	
08/967, 148	November 10, 1997	

And I hereby appoint

John P. White (Reg. No. 28,678); Christopher C. Dunham (Reg. No. 22,031); Norman H. Zivin (Reg. No. 25,385); Jay H. Maioli (Reg. No. 27,213); William E. Pelton (Reg. No. 25,702); Robert D. Katz (Reg. No. 30,141); Peter J. Phillips (Reg. No. 29,691); Wendy E. Miller (Reg. No. 35,615); Richard S. Milner (Reg. No. 33,970); Robert T. Maldonado (Reg. No.38,232); Paul Teng (Reg. No. 40,837); Richard F. Jaworski (Reg. No. 33,515); Alan J. Morrison (Reg. No. 37,399); Mark A. Farley (Reg. No. 33,170); Pedro C. Fernandez (Reg. No. 41,741); Gary J. Gershik (Reg. No. 39,992); Alan D. Miller (Reg. No. 42,889); Frank Bruno (Reg. No. 46,583); and Christine S. Nickles (Reg. No. 51,103)

and each of them, all c/o Cooper & Dunham LLP, 1185 Avenue of the Americas, New York, New York 10036, my attorneys, each with full power of substitution and revocation, to prosecute this application, to make alterations and amendments therein, to receive the patent, to transact all business in the Patent and Trademark Office connected therewith and to file any International Applications which are based thereon under the provisions of the Patent Cooperation Treaty.

Declaration and Power of Attorney

I hereby claim the benefit under Title 35, United States Code, Section 119(e) of any United States provisional application(s) listed below:

Provisional Application No.	Filing Date	Status

I hereby claim the benefit under Title 35, United States Code, Section 120 of any United States Application(s), or Section 365(c) of any PCT International Application(s) designating the United States listed below. Insofar as this application discloses and claims subject matter in addition to that disclosed in any such prior Application in the manner provided by the first paragraph of Title 35, United States Code, Section 112, I acknowledge the duty to disclose to the United States Patent and Trademark Office all information known to me to be material to patentability as defined in Title 37, Code of Federal Regulations, Section 1.56, which become available between the filing date(s) of such prior Application(s) and the national or PCT international filing date of this application:

Application Serial No.	Filing Date	Status
09/100,631	June 18, 1998	
09/100,763	June 18, 1998	
09/100,529	June 18, 1998	
09/100,762	June 18, 1998	
09/100,521	June 18, 1998	
08/976,741	November 24, 1997	

And I hereby appoint

19 John P. White (Reg. No. 28,678); Christopher C. Dunham (Reg. No. 22,031); Norman H. Zivin (Reg. No. 25,385); Jay H. Maioli (Reg. No. 27,213); William E. Pelton (Reg. No. 25,702); Robert D. Katz (Reg. No. 30,141); Peter J. Phillips (Reg. No. 29,691); Wendy E. Miller (Reg. No. 35,615); Richard S. Milner (Reg. No. 33,970); Robert T. Maldonado (Reg. No.38,232); Paul Teng (Reg. No. 40,837); Richard F. Jaworski (Reg. No. 33,515); Alan J. Morrison (Reg. No. 37,399); Mark A. Farley (Reg. No. 33,170); Pedro C. Fernandez (Reg. No. 41,741); Gary J. Gershik (Reg. No. 39,992); Alan D. Miller (Reg. No. 42,889); Frank Bruno (Reg. No. 46,583); and Christine S. Nickles (Reg. No. 51,103)

and each of them, all c/o Cooper & Dunham LLP, 1185 Avenue of the Americas, New York, New York 10036, my attorneys, each with full power of substitution and revocation, to prosecute this application, to make alterations and amendments therein, to receive the patent, to transact all business in the Patent and Trademark Office connected therewith and to file any International Applications which are based thereon under the provisions of the Patent Cooperation Treaty.

09856200.010303

Please address all communications, and direct all telephone calls, regarding this application to:

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I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

1-00

Full name of sole or first joint inventor: Peter D. Kwong

Inventor's signature: Peter Kwong

Citizenship: USA Date of signature: 10 October 2002

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2-00

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Inventor's signature: [illegible]

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3-00

Full name of joint inventor (if any): Joseph G. Sodroski

Inventor's signature: Joseph G. Sodroski

Citizenship: USA Date of signature: 11/26/02

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Declaration and Power of Attorney

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

Full name of sole or first joint inventor Richard T. Wyatt

Inventor's signature Richard T. Wyatt

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Inventor's signature ___

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Full name of joint inventor (if any) ___

Inventor's signature ___

Citizenship ___ Date of signature ___

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